

1995

Investigation in the Theory of Stochastic Processes.

Xiao Liang Li

Louisiana State University and Agricultural & Mechanical College

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INVESTIGATION IN THE THEORY OF STOCHASTIC PROCESSES

A Dissertation

**Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
in partial fulfillment of the
requirements for the degree of
Doctor of Philosophy**

in

The Department of Physics and Astronomy

**by
Xiao Liang Li
B. S., Fudan University, 1985
May 1995**

UMI Number: 9538747

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To my parents

ACKNOWLEDGMENTS

I would like to express my sincere appreciation and gratitude to my research advisor, Boyd Prof. R. F. O'Connell, for his continuous help, guidance, and encouragement during this research.

Appreciation also goes to the publishers of Physical Review A and American Journal of Physics, and the North-Holland Physics Publishing Division of Elsevier Science Publishers, for their permission to use the reprints in this dissertation. In addition, I am grateful to A. Jackson for her help in preparing the preprint contained in Chapter III, Section 5.

This research was partially supported by the U. S. Office of Naval Research and by the U. S. Army Research Office.

PREFACE

This dissertation consists of three chapters: Chapter I serves as a general introduction to stochastic processes in physics; Chapter II deals with some applications of the generalized quantum Langevin equation approach for a one-dimensional dissipative system; and Chapter III extends the work to the three-dimensional quantum dissipative system of a charged particle placed in an external magnetic field. The text contains reproduction of the body text of six research papers (four reprints of published papers and two preprints of ones to be submitted) as individual sections in Chapters II and III, with their abstracts incorporated in Introductions to Chapters II and III. To accommodate the format of this dissertation, they are edited to place both their authorships and acknowledgments in the footnotes of their respective sections and their references are merged into the overall bibliography of this dissertation. Written permissions from the publishers are included in the Appendix to this dissertation.

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ABSTRACT

In Chapter I of this dissertation, we present a pedagogical introduction to the basic concepts of stochastic theory and review the progress made as well as the outstanding unsolved problems in the field.

For the rest of this dissertation, we use a generalized quantum Langevin equation (GLE) approach to investigate various properties of quantum dissipative systems.

In Chapter II, calculations for the displacement and random force correlation functions for Brownian motion are generalized to the case of an arbitrary heat bath for a damped harmonic quantum oscillator. The mean square displacement of such an oscillator is then evaluated for both Ohmic and blackbody radiation heat baths, to determine the effects of many parameters on the localization of the oscillator.

In Chapter III, the formalism is extended to the Brownian motion of a charged particle in an external magnetic field as well as in a potential. The influence of the magnetic field on the memory function and random force is determined, with the blackbody radiation heat bath analyzed as a special case. For a charged harmonic oscillator, the generalized susceptibility is obtained, which enables us to derive the symmetrized position correlation functions using the fluctuation–dissipation theorem. In addition, we obtain the free energy of the system by generalizing the “remarkable formula” of Ford, Lewis, and O’Connell. Explicit calculations are performed for Ohmic and blackbody radiation heat baths. Furthermore, the effect of dissipation on the localization of the oscillator in an Ohmic heat bath at zero temperature is shown to differ qualitatively from that without the magnetic field. Finally, we formulate retarded Green’s functions and symmetrized position correlation functions for the oscillator, reach some general conclusions, and

make explicit calculations for the Ohmic heat bath. For the special case of Brownian motion at both zero and nonzero temperatures, we prove two general asymptotic relations between the retarded Green's functions and the displacement correlation functions, which we use to evaluate the long-time behaviors of the latter from those of the former, for both the Ohmic heat bath and a rather general class of heat baths discussed extensively in the literature.

CHAPTER I

INTRODUCTION TO STOCHASTIC PROCESSES

1. Some Basic Concepts and Problems in Stochastic Physics

The objective of theoretical physics up to the end of the last century can be summarized as the study of differential equations and the modeling of natural phenomena by *deterministic* solutions of these differential equations. By deterministic, we mean a time evolution of a system such that the future state of the system is uniquely determined by its past (and actual) state. The prevalent illusion then was that if only all initial data could be specified, one might be able to predict the future with certainty.

Such an illusion has been proven wrong, for unpredictability can enter into physics in three ways. First, the beginning of this century marked the arrival of a new physics, quantum mechanics, which has in its foundation an essentially statistical element [1]. Quantum uncertainties are inherent in the basic theory, as expressed by the Heisenberg uncertainty principle, and occur even in a pure state. Second, the phenomenon of *chaos* has more recently been discovered, in which even ostensibly simple systems of nonlinear differential equations can lead to basically unpredictable behavior. To be precise, the future of such a system could still be forecast given its initial conditions exactly. However, uncertainty in the initial conditions is unavoidable for real systems and, for a chaotic system, it is magnified so rapidly that no practical predictability is feasible [2]. For such a system, unpredictability is an integral part of the theory.

Stochastic processes in classical systems, on the other hand, originate from *statistical fluctuations*, which always reflect a lack of knowledge about the exact microscopic state of the system [3]. This is the third way in which unpredictability can enter into physics.

Many natural phenomena depend on time in such a complicated way that they are far beyond the reach of calculation and often even of observation. Nevertheless, they usually possess some average features that can be observed and do obey simple laws. Therefore, the application of probability in physics finds its justification in our ignorance of the precise microscopic states and, despite this ignorance, in the possibility of detecting regularities in the macroscopic behavior and of further formulating them in general laws. Although a large system itself consists of myriad discrete particles, it may still be describable, through “coarse-graining” in phase space, in terms of a few macrovariables of interest. This corresponds to an enormous reduction in information, which necessarily requires a probabilistic description. The consequent loss of knowledge about the microscopic degrees of freedom gives rise to “intrinsic” fluctuations of the microvariables [4,5]. This internal noise is inherent in the very way in which the state of the system evolves and thus can not be separated from its equations of motion. In addition, the external forces in the equations of motion, which describe the response of the system to the outside perturbation, have to be considered as fluctuating quantities as well, since they are produced by other macroscopic systems. They impose “external” fluctuations on an otherwise deterministic system [6].

The study of fluctuation phenomena in science began in essence in 1827 when the Scottish botanist Robert Brown discovered under his microscope very animated, irregular motion of small pollen grains floating on water [7]. The observed phenomena took the name *Brownian motion* in recognition of his pioneering work. By showing that the motion was present in any suspension of fine particles of colloidal size in a liquid medium, he ruled out any specifically organic origin of this motion. Brownian motion always exists, even in thermal equilibrium, as a fluctuation. It needs only the right circumstances—low mass, weak binding to a nucleus or otherwise, and small frictional forces—to make its appearance.

It became fairly apparent by the turn of the century, even when atomic theory had not yet been fully established as reality, that Brownian motion has its origin in molecular motion. Several experimental findings had begun to shed light on this connection. It was known, for example, that the smaller a particle's size, the more rapid its Brownian motion. Increasing temperatures of the fluid medium was also shown to cause more agitated Brownian motion. Such effects were recognized as being consistent with the kinetic theory of gases soon after its development in the 1870's [8].

However, it was the celebrated paper of A. Einstein in 1905 [9] that first turned the study of Brownian motion into a conclusive, observational method for confirming the atomic theory of matter. Even though Einstein did not know that Brownian motion had already been observed long ago when he first came upon the idea to verify directly the atomic concept, his work finally convinced people of the truth of the theory of heat based on molecular motion and, in doing so, ushered in the modern physics of the twentieth century. His solution to the problem of Brownian motion builds on two premises. First, the Brownian motion is recognized as being caused by the exceedingly frequent and statistically independent impacts on the pollen grain of the ceaselessly moving molecules of liquid in which it is immersed. Second, the motion of these molecules is so complicated that its effect on the pollen grain may be described only *probabilistically* in terms of these impacts. The first point results in a *Gaussian* distribution of the displacement for the Brownian particle due to the *central limit theorem* [10], whereas the second implies that it is a *Markovian* process as well because correlation between successive impacts lasts only for the mean free time of such molecular motion, which is short compared with the time scale of the Brownian motion. Fluctuations of this kind demand a new statistical formulation of them as an intrinsic part of the time evolution of the system, in contrast to the description of possible states and the probability of their realization as adopted in the kinetic theory of gas. Although Rayleigh [11] might be considered by some to be the first to ponder a stochastic

description in the modern sense, for all practical purposes, Einstein's theory about the nature of Brownian motion has to be regarded as the commencement of *stochastic modeling* of natural phenomena.

A similar explanation of Brownian motion was independently developed by Smoluchowski [12], who was responsible for much of the later systematic development and the experimental verification of the theory. The measurement of the mean square displacement of particles in Brownian motion helped determine, for the first time, several important physical constants: the magnitude of Avogadro's number and the masses of atoms and molecules [13]. The theory of Brownian motion was further advanced by Langevin [14], Uhlenbeck and Ornstein [15], Chandrasekhar [16], and many others. An excellent review of the classical theory was presented by Wang and Uhlenbeck [17]. Ref. 18 collects many original and important contributions; more recent (and more mathematically oriented) contributions may be found in Ref. 19. Since then the study of Brownian motion has had wide consequences for physics, chemistry, and mathematics. It has also deepened the theoretical understanding of thermodynamic principles, which had previously been established based on oversimplified empirical generalizations. Application of the mathematical techniques for the general investigation of probabilistic processes has contributed to the understanding of the dynamics of star clustering [16], the drag force in viscous fluids and dissipation in turbulence [20], the evolution of biological and ecological systems [21], and the behavior of financial markets [22].

The path of a Brownian particle immersed in a fluid reflects, in fact, a double random effect. It is randomized by the fluctuations in velocities of nearby molecules (the Uhlenbeck–Ornstein process [15]). Moreover, because the microscope essentially reveals only the effects of relatively large local fluctuations, the observed motion does not expose the whole complexity of the true path. Each increase in the magnification would bring out a rugged structure to parts of the trajectory of the particle initially appearing to be straight

lines, as the effects of bombardment by progressively smaller clusters of molecules could be detected. The trail of a Brownian particle was one of the first natural phenomena recognized as being effectively self-similar at every magnification, the hallmark of the geometric objects called *fractal curves* [23].

The mathematical theory of stochastic processes (also called *Wiener processes*) was initiated by N. Wiener for the study of Brownian motion [24]. It is fundamental to the description of systems that do not behave in a deterministic way, but instead display statistical fluctuations in the system variables. Such systems occur in almost every discipline of science, particularly in physics and the applied sciences [25].

A stochastic process is a time evolution of random variables that, in physical parlance, may be regarded as an “ensemble” of sample functions or realizations of the process as observed in experiments. In many cases, the stochastic process has no long term memory. A highly restrictive conjecture then amounts to the assumption that it has no memory at all. Such a purely random process is called a *white noise* process because its spectrum is flat (i.e., independent of frequency), an example of which is the shot noise effect [26]. A much less narrow hypothesis defines the so called Markovian processes, the evolution of whose probability in the next instant is determined by its present state. As a result, the whole hierarchy of multiple-time distribution functions for a Markovian process is generated by its two-time transitional probability distribution function satisfying the Chapman–Kolmogorov equation. This represents an enormous simplification, the justification for which relies on the separation of the time scales of microscopic and macroscopic motions. If all slow variables of the system are to be included among the macroscopic variables, the Markovian description of the stochastic process should be justified for macroscopic times. The Boltzmann equation describes a Markovian process, while an ideal Brownian motion is another good example of the Gaussian–Markovian process.

The central idea of statistical mechanics for a stationary process is the substitution of an actual system by a suitably chosen ensemble of systems, all having the same equations of motion but different initial conditions. The ensemble merely serves as a convenient tool for visualizing the probability distribution, which in equilibrium statistical mechanics is postulated as being equal for every microscopic state. In this picture, every physical quantity has effectively become a stochastic variable, whose ensemble average may be used in place of its time average that is directly observable [27]. This is the ergodic hypothesis proposed by Boltzmann in order to support the equal weight principle, the justification of which still remains an outstanding problem in equilibrium statistical mechanics.

For nonequilibrium processes, the probabilistic method must be stochastic, describing the temporal evolution of the probability for the macrovariables that adequately characterize the coarse-grained states of the system under study. Switching from microscopic dynamics to a stochastic description is sometimes termed stochastization, an essential part of which is the bold assumption called Stosszahl Ansatz (assumption for the collision frequency) or random phase approximation [8]. In practice, this statistical hypothesis of “molecular chaos” involves repeatedly averaging out the irrelevant variables at successive time scales. Furthermore, to obtain a simple and clear description of macroscopic equations, it is necessary to simultaneously make coarse graining in both space and time by limiting the precision of spatial and temporal measurements successively [28]. These procedures combine to effectively eliminate the irrelevant (rapidly varying) microvariables and lead to macroscopic differential equations for the evolution of the remaining (slowly varying) macrovariables themselves, with small deviations identified as fluctuations. This approach to stochastic processes may be denoted as mesoscopic [6], which is more detailed than the macroscopic description by including fluctuations but has abbreviated the microscopic equations through sequential averagings. The profound consequence of this assumption is manifest as the resulting macroscopic and mesoscopic processes in nature are

irreversible, in which entropy can only increase, while the underlying microscopic equations are reversible in time [29]. The true cause of this difference is still a fundamental problem waiting for a satisfactory answer, even though chaotic dynamics may render Boltzmann's statistical hypothesis unnecessary in some cases [30].

When stochastically modeling a physical system, one has successive stages of coarse graining depending on the incompleteness of the description. The Boltzmann equation is the oldest example of stochastic modeling, while the hydrodynamic equations for a gas, which can be derived from the former, constitute a more crude description. A class of stochastic equations more general than the Boltzmann equation is the so called *master equation* obeyed by the transitional probability distribution function of any stationary Markovian process [31]. The master equation is a differential version of the Chapman–Kolmogorov equation, but is more convenient to handle mathematically and has a more direct physical interpretation. It determines the evolution of all Markovian systems over very long time intervals.

Fluctuation phenomena in statistical mechanics dominate on a microscopic scale. On the other hand, the effects of fluctuations in macroscopic variables are usually negligible, except in certain situations in which they may be important [32]. Typical examples of the latter include the scattering of light or of particles by an opaque liquid system [16], critical fluctuations near phase transitions and instabilities [33], and the decay of metastable states [34].

The notion of Brownian motion resulting from the statistical fluctuations amid the microstates of a thermodynamic system had even greater significance for the study of *nonequilibrium systems* than for that of systems in equilibrium. The mathematical treatment of nonequilibrium thermodynamics can be traced back to a *stochastic differential equation* describing the motion of a particle in a viscous fluid that was formulated by the French physicist Paul Langevin in 1908 [14]. Stochastic differential equations are simply

differential equations whose coefficients are random functions of the independent variables with predetermined stochastic properties. They serve to describe systems with fluctuations caused by an external agent. Langevin's continuous time approach is to be contrasted with Einstein's original derivation using the discrete time assumption. A primary feature of the *Langevin equation* is the separation of the total force arising from the particle's environment into two components that have distinctly different time scales. The frictional force, inversely proportional to the self-diffusion constant, has a time scale much longer than that for the random force determined by the mean time between atomic collisions. The range of validity of a Langevin-type equation is thereby prescribed by the time scale of the random force; the simple Langevin equation is valid for the description of processes that occur on a time scale much larger than the mean time between atomic collisions. Langevin's approach is more direct, offering a natural way of generalizing a microscopic dynamical equation to a stochastic one. Its solid mathematical foundation was established more than forty years later by K. Itô [35] based on his formulations of the calculus of stochastic differentials and of stochastic differential equations.

For Markovian–Gaussian processes such as the Brownian motion, complete information is furnished by the transitional probability distribution function of the particle's velocity satisfying the *Fokker–Planck* (FP) equation [36]. The Markovian property of the driven process comes from the white noise character of the random force, whereas the Gaussian assumption leads to the Fokker–Planck description in which the random force is eliminated from the equation, leaving only its spectral function of intensity. The FP equation is a special type of the master equation but, on the other hand, a generalization of the diffusion equation. It describes a large class of very interesting stochastic processes in which the system has a continuous sample path [15]. It can be applied even for nonlinear as well as nonstationary systems, though it is limited to Markovian cases where the underlying process is both white and Gaussian. By comparison, the Langevin equation can be

easily solved by harmonic analysis (i.e., the Fourier transformation method) regardless of the spectral form of the random force, but its value is severely limited if the basic driving stochastic process is not linear.

In 1931 L. Onsager observed that, by a mere change in notation, Langevin's equation could statistically describe an *irreversible process* [37]. He discovered that if the velocity of the particle in Langevin's equation is replaced by the deviation of a thermodynamic quantity from its equilibrium value and if the frictional force on the particle is replaced by the drift of a thermodynamic system toward its equilibrium state, then the resulting equation can be used to study the effect of thermal fluctuations on irreversible processes. This remarkable mathematical maneuver belies a deep resemblance between the motion of the particle and the decay of a nonequilibrium state. Over a time much longer than that for a fluctuation to subside, the average course of decay could be presumed to be given by the phenomenological laws of nonequilibrium thermodynamics. This assumption led him to an exposition for the heat conductivity in terms of a correlation function of energy flux. Since fluctuations are of microscopic origin dynamically, they have time-reversal symmetry. This in turn permitted him to prove the reciprocity of the heat conductivity tensor and, in general, of a set of kinetic coefficients for an anisotropic substance. This theorem later served as the foundation of nonequilibrium thermodynamics as developed by Prigogine and others [38].

The traditional approach to nonequilibrium statistical mechanics is the so called kinetic method employing the Boltzmann equation. The relevant time and energy scales for any process in a liquid or gas are the collision time τ_c , the mean free time τ_m , and the ratio of the average potential to kinetic energies. In condensed matter not too dense, there is distinct separation between the time and energy scales. Processes that occur on a time scale much smaller than τ_c must be governed by microscopic equations, whereas those that arise on a time scale much larger than τ_m are appropriately described by continuum or

hydrodynamic equations. For example, a treatment of Brownian motion as diffusion is possible only for a time scale much larger than the mean free time τ_m and a spatial scale much larger than the mean free path l . The intermediate time region is usually referred to as the kinetic regime. The kinetic method assumes that stochastization can be accomplished, for example, with a Boltzmann-type equation or a Markovian equation for an appropriate probability distribution function. It is applicable only for a system having a sufficiently amenable structure, and only if we confine ourselves to a certain class of physical properties corresponding to the required level of crudeness for stochastization. However, it is unsuited to dense systems of interacting particles. Within its own range of validity, though, such a method is very powerful indeed and can be utilized for nonlinear systems as well.

An alternative approach to nonequilibrium statistical mechanics is usually called the linear response theory [28,39] in which the stochastization, if ever made, is instituted at a later stage after the linearization procedure. The key ingredient of this theory is the *fluctuation-dissipation theorem* (FD) [5,40], from which many fundamental laws such as the Kramers-Kronig dispersion formula and Onsager's reciprocity could be derived. The FD theorem shows clearly the intimate connection between fluctuations in equilibrium and dissipation (the nonequilibrium properties of a system), which is expected since they both originate from the same random molecular motion. Thus the linear response theory has roughly the same range of validity as that for equilibrium statistical mechanics. The root of the FD theorem may be traced back to the Einstein relation linking the diffusion coefficient with the viscosity [9]. Its present form was first presented by Nyquist [41], who based his derivation on a thermodynamic consideration of detailed balance to demonstrate that the random fluctuations in voltage across a resistor (thermal or Nyquist noise) are determined by its impedance, as measured by Johnson [42]. The quantum formulation of the FD theorem appeared in the celebrated paper of Callen and Welton [43]. Its most recent version is

the Green–Kubo formula [4,39] that relate transport coefficients to integrals of appropriate correlation functions. The usefulness of the linear response theory and, in particular, the FD theorem is further aided by development of the Green’s function method in modern quantum statistical mechanics [44], which has greatly facilitated the evaluation of response functions for many-body systems.

The theory of stochastic processes also found its application in Feynman’s path integral formulation of quantum mechanics [45]. According to Feynman, quantum mechanics is not so much a new probability as it is a new mechanics. The probabilities appearing in quantum mechanics are of the same type as those found in any other statistical theory; what distinguishes them is the mathematical model of their computation. After the invention of the Feynman path integral, many attempts have been made to give it a precise mathematical interpretation [46]. A very successful approach has been to stress the connection of the Feynman path integral with the integrals associated with stochastic processes [47]. Nelson [48] noticed that the imaginary-time Schrödinger equation may be reformulated in terms of a stochastic differential equation, namely a diffusion equation, whose solution justifies the introduction of Gaussian processes at least on a heuristic level. For the real-time evolution, one is referred to other classical processes, specifically the Poisson processes. Nelson’s theory of quantum mechanics may be more than a beautiful mathematical tool. It could be more fundamental than other formulations, serving as the spring board for a whole new mechanics of which quantum mechanics will only be a special type [49].

The study of stochastic processes has recently been combined with that of chaotic dynamics [50]. Stochastic modeling of deterministic differential equations leads to the important question of the stability of their solutions to an additive noise term in the equations, the characterization of which by means of the Lyapunov exponent distinguishes between chaotic processes and regular stochastic processes perturbed by fluctuations [51]. The current research on dissipative dynamical systems has mostly been motivated by the attempts

to account for various phenomena observed in real fluid dynamical experiments including, particularly, the enormously complex issue of fluid dynamical turbulence [52].

Over the last three decades the problem of describing stochastic processes in a quantum system has attracted renewed interest [53]. Here, the fundamental difficulty is how to reconcile dissipative equations of motion with the processes of quantization. This obstacle stems from the facts that the standard procedures of quantization depend on the existence of either a Hamiltonian or a Lagrangian function for the system of interest, and that a Langevin-type equation of motion can not be derived by merely applying Hamilton's principle to any Hamiltonian or Lagrangian for the system itself that does not explicitly depend on time. Since Pauli's seminal work in 1928 [54], a great variety of approaches aiming at a consistent quantum mechanical description of dissipation have been proposed. The most obvious of them all is the simple use of time-dependent functions that would allow us to apply the standard schemes of quantization directly. Historically, Caldirola [55] and Kanai [56] were the first to employ a time-dependent mass chosen such that a frictional term appears in the classical equation of motion. However, this method was shown to inevitably run afoul with the Heisenberg uncertainty principle [57], and it is now generally believed that dissipation cannot satisfactorily be described just by a time-dependent mass.

Many other approaches to dissipative quantum systems were also explored, the majority of which fall into two main categories. They either seek new rules of quantization or attempt the system-plus-reservoir approach.

Among the first class, Dekker [58] developed a canonical quantization procedure for complex variables, thereby reproducing some interesting results such as the Fokker-Planck equation for the Wigner distribution function. However, some *ad hoc* suppositions in his work like the invocations of different noise sources in the equations of position and momentum are rather controversial. Kostin [59] introduced another strategy using a non-linear Schrödinger equation. Besides violating the superposition principle of quantum

mechanics, this theory is beset by some very doubtful results like stationary damped states. Yasue [60] later deduced the same nonlinear Schrödinger equation based on Nelson's stochastic quantization procedure [48], which is pertinent because in Nelson's quantization scheme only the equation of motion itself is involved instead of Hamiltonians or Lagrangians. The chief concern here appears to be the correctness of Nelson's theory. Along with lacking clear theoretical foundations, all these approaches can at best duplicate only known results for very special instances, like linear systems in the limit of weak dissipation.

A more natural (and more successful) approach is to regard the system and its environment as the constituents of a conservative composite system obeying the standard rules of quantization. It was pioneered by Senitzky [61] in his work on the damping of electromagnetic field modes in a cavity, in which the interaction of the system of interest with a reservoir is explicitly taken into account. He was the first to propose, with the elimination of bath operators, a quantum Langevin equation in the Heisenberg picture. However, his treatment was restricted to the Markovian process in the weak coupling limit (the Born approximation) and contains a serious error in that he used a power spectrum of white noise for the fluctuating force instead of the Planck spectrum of quantum noise [62]. A correct formulation in this regard was first presented by Ford, Kac, and Mazur (FKM) [63]. Senitzky's method was later advanced by Mori [64] who showed that a microscopic equation of motion can generally be transformed into the form of a generalized quantum Langevin equations (GLE) for operators by projecting the operators of the composite system onto the set of macroscopically relevant operators. In this formalism, it is crucial to span the subspace with the complete set of macrovariables. Otherwise, the fluctuating force would contain slowly varying components, rendering the separation of time scales incomplete. An excellent review of the generalized Langevin equation approach has been given by Gardiner [65]. An alternative commonly used method, along the same line of

system plus reservoir, utilizes successfully, in the Schrödinger picture, associated generalized master equations of the density operator [66 – 68] to investigate dissipative phenomena, for example, in quantum optics and spin relaxation theory [34,69 – 72].

Still another approach to the problem of quantum dissipation centers on seeking to generalize the classical Langevin equation for a Brownian particle to the quantum domain [63]. This technique was used by Koch *et al.* [73] to analyze the low-temperature performance of Josephson junctions. Its theoretical foundation was discussed by Benguria and Kac [74] and Ford and Kac [75], who argued that only with the general retarded form of the Langevin equation, together with the Planck power spectrum and the Gaussian property for the random force, does one have the correct approach to a unique equilibrium state.

Instead of trying to quantize the dissipative system itself, the most fruitful approach strives to consider it from the very beginning as interacting with a complex environment. It is precisely this interaction that gives rise to dissipation. Since the complete “universe” formed by the system together with its surroundings may be regarded as closed, the standard quantization procedures are of course applicable to the coupled systems. Thereafter the environment coordinates may be eliminated to obtain a closed equation of motion for the dissipative system itself. To this end, one needs to choose a sufficiently simple model for the system–reservoir interaction. This step is unavoidable because for many complex systems, a clear understanding of the microscopic origin of dissipation is often unavailable. Nevertheless, it might sometimes be possible to acquire knowledge of the power spectrum of the stochastic force in the classical regime. Therefore it is necessary to set up tractable models that could reproduce the classical results for Brownian motion in the high-temperature limit [76].

The simplest model of a dissipative quantum system that one can imagine is a particle (in the general sense) coupled to a passive heat bath linearly through its displacement. The heat bath may well be approximated as linear in its coordinates if any one particular

degree of freedom of it is only weakly disturbed by the particle. This linearity assumption is physically reasonable for a geometrically macroscopic heat bath, for which the interaction of the particle with any one bath degree of freedom is inversely proportional to the volume of the bath and hence very small. However, the influence of the heat bath on the particle is not necessarily weak as well, since the total number of bath degrees of freedom coupled to the particle is extremely large. Such a linear-coupling model corresponds to a heat bath composed of harmonic oscillators, with the associated statistics strictly Gaussian [77]. It has been introduced and discussed systematically by Ullersma in a series of four papers [78]. Early studies for a harmonic potential include the works by Rubin [79] for classical systems, and by Senitzky [61] and Ford *et al.* [63] for quantum systems. Zwanzig *et al.* discussed this model for a nonlinear potential as well as the associated nonlinear Langevin equation in the classical regime [76,80]. It was later revived and generalized to nonlinear dependence on the particle's coordinate, and applied to the problem of dissipative quantum tunneling by Caldeira and Leggett [77] employing the influence-functional technique of Feynman and Vernon [81]. Since then, the model has usually been called the Caldeira–Leggett model in the literature.

However, the original Ullersma model and its variants contain a serious flaw: they do not have a lower bound on the energy spectrum that is necessary to guarantee the existence of unique thermal equilibrium states. This defect has plagued many results in the field. Though it was recognized and remedied by many authors at later stages of their calculations using various procedures, the corrections have not been made consistently. The correct starting point was provided by Ford, Lewis, and O'Connell (FLO) [82] using what they called the independent-oscillator (IO) model, the Hamiltonian of which differs from that of the Ullersma model by extra terms of second order in coordinates of the bath oscillators such that it is a sum of complete squares and hence positive definite. The approach of FLO to the dissipative problem of quantum systems is the generalized quantum Langevin

equation (GLE) consistent with fundamental physical principles and, further, independent of any specific model [82 – 84]. They have employed this technique systematically in solving many important physical problems, including the first correct treatment of the blackbody radiation (BBR) heat bath [83,85 – 88]; the first correct derivation of the normal-mode frequencies for the coupled dissipative system [89]; the first calculation of free energies for a dissipative oscillator [83,88,89]; transport theory [84]; dissipative quantum tunneling in Ohmic [90] and BBR [91] heat baths; canonical commutator and mass renormalization [92]; the equation of motion of a radiating electron and the problem of the electron's structure [93,94] and its relativistic extension [95]; and dissipation in a squeezed-state environment [96].

CHAPTER II

ON SOME APPLICATIONS OF THE GENERALIZED QUANTUM LANGEVIN EQUATION APPROACH

1. Introduction to Chapter II

Chapter II of this dissertation is concerned with the application of the generalized quantum Langevin (GLE) to the investigation of some properties of one-dimensional (1D) quantum dissipative systems.

The problem of open quantum systems has been around since the dawn of quantum mechanics [97]. It is fundamental to many fields as diverse as solid-state physics, chemical physics, biophysics, quantum measurement theory, quantum optics, nuclear and particle physics [25]. Despite the success of quantum mechanics in explaining physical processes on an atomic or sub-atomic level, a well-known enigma remains about the transition between quantum mechanics and the macroscopic world around us, which is governed by the laws of classical mechanics. This relation is unique in that although quantum mechanics comprises Newtonian mechanics as its limiting case, at the same time it requires this limiting case for its own formulation based on the concept of measurement (i.e., the interaction of a quantum object with a classical measuring apparatus) [98]. Naturally, the question arises of how quantum theory extrapolates to macroscopic systems, which has to be answered experimentally.

The subject has gained renewed interest recently with the advent of modern lithographic techniques for fabricating various microstructures in a controlled manner. In the low-temperature regime, the dissipative influence of a heat bath on the motion of a quantum particle has been found to give rise to such novel features as the exponential suppression of tunneling by dissipation [77,90,91], dissipative quantum phase coherence

[99 – 103], long-time tails in correlation functions [104], and dissipative phase transitions [105,106].

The quantum particle under study could be microscopic, e.g., a single atom [83], or macroscopic, e.g., a magnetic flux trapped in the current-biased Josephson Junction or the superconducting ring of a *rf* superconducting quantum interference device (*rf* SQUID) at very low temperatures (a few millidegrees above absolute zero) [100,102,107,108]. The issue of quantum mechanics for macroscopic systems has been stimulated strongly by Leggett's discussion of the validity of quantum mechanics at the macroscopic level [109]. Further impetus was provided by the work of Caldeira and Leggett [77] on quantum tunneling in the presence of dissipation at zero temperature. The basic difficulty in applying quantum mechanics to macroscopic objects stems from the fact that even for a macroscopic object describable by a single collective variable, which may be justified for specific models [110], there is invariably an environment arising from all the microscopic degrees of freedom [109]. Therefore, the "particle" and its surrounding medium have to be regarded as the constituents of a conservative composite system obeying the standard rules of quantization [61,63,64,66 – 8]. In this account, dissipation comes about naturally as a result of the transfer of energy from the "small" system composed of a single particle to the "large" reservoir. For a particle not in equilibrium with the heat bath, its kinetic energy, once transferred, disappears into the heat bath and will not be given back within any physically relevant time, leading to friction in the motion of the particle.

The generalized quantum Langevin equation (GLE) for Heisenberg operators furnishes a potent and physically appealing approach to this kind of problems, as pointed out by Ford, Lewis and O'Connell [82]. It is a complete macroscopic description of the quantum dissipative system, with the fast degrees of freedom of the environment being integrated out [64], that can be formed exactly and generally, using such fundamental physical principles as causality and the second law of thermodynamics. Although it is

model-independent, it may conveniently be accommodated by the simple independent-oscillator (IO) model of the heat bath [75,82,111,112]. This model is a very simple one in which the quantum particle under study is attached by springs to a large number of heat-bath particles. It was shown explicitly in Ref. 82 that this model is equivalent to the velocity-coupling model [82], the FKM model [63], the Lamb model [113], the translationally invariant version of the Caldeira–Leggett model required for a free Brownian particle [111], and the Schwabl–Thirring model [114]. Other superficially similar but defective linear-coupling models are the Ullersma model that appears frequently in the literature [78], and the rotating-wave approximation often used in works on quantum optics [57]. These are all oscillator-bath models in which the coupling to the particle is through a term linear in the particle displacement. However, they all have a serious defect in that for a free particle, their energy spectrums are not bounded from below. This implies that for these models, there is no thermal equilibrium state and hence the heat baths constructed are not passive, in direct violation of the second law of thermodynamics [82]. In practice, they are usually rectified by adding at some later stage of derivation a “counter term” [77], by imposing a “positive condition” on the external potential [78], or by requiring the underlying Hamiltonian to be translationally invariant in space for a free Brownian particle [111]. These repairs are not unique and have led to persistent errors in the literature in applying the linear-coupling model and its variants.

The construction of the IO model, on the other hand, guarantees that the corresponding Hamiltonian operator has a lower bound on its spectrum thus ensuring the existence of unique thermal equilibrium states. The passivity condition of the heat bath, that the system will eventually relax to a sole thermal equilibrium state, is secured by requiring the heat bath embrace a continuous spectrum of oscillator frequencies and coupling constants down to the zero frequency (and thus an infinite number of degrees of freedom in the heat bath), so that the Poincaré recurrence time is infinite [61]. Other approaches

along the same line of system-plus-reservoir include the path integral formulation [77,115,116] and an application of the quantum Fokker-Planck equation [57]. All these methods have their own advantages. The strength of the GLE approach lies in its simplicity and generality in carrying out calculations, at least for linear systems, and in interpreting relevant results.

The standard experimental techniques for probing dynamical processes in a complex many-body system employ quasielastic and inelastic scattering of electrons, neutrons, photons, or x-rays off a sample; and the energy loss of a charged particle traveling through the system, due to its interaction with the charges in the system. The system's response to these external driving forces, analyzed from the line shapes of the corresponding spectra, yields vital information about the dynamical behavior of the spontaneous fluctuations and may be rigorously formulated in terms of time correlation functions. Correlation functions are therefore indispensable for the theoretical interpretation of experiments in condensed matter physics. Moreover, they are amenable to calculation with realistic, many-particle models [117]. For linear processes, all higher-order correlation functions can be factorized into summation of simple pair correlation functions due to the Gaussian properties of the underlying stochastic processes [63,78,82,104].

In a paper entitled "Correlation in the Langevin theory of Brownian motion" [118], the body text of which constitutes Section 2 of this dissertation, the time correlation function of the displacement and the random force for a quantum Brownian particle in an Ohmic heat bath is calculated by using the GLE. In the high-temperature regime, its equal-time value reduces to the classical result [14,119]. The generality of the GLE approach enables one to easily extend the calculations to the quantum domain and to the case of an arbitrary heat bath. Memory effects of the environment are illustrated by consideration of the blackbody radiation heat bath. In addition, extension is made to the case

of a damped harmonic oscillator to examine the effect of a harmonic confining potential on the time correlation function of its displacement and the random force. The formalism thus presented may easily be applied, for example, to analyze the energy balance for a dissipative system [120]. It is shown there that the work done by the fluctuation force on a quantum particle exactly compensates the energy lost by the particle due to the frictional force at any temperature (including absolute zero), a necessary condition for maintaining equilibrium. Besides a brief history of the theoretical works on stochastic processes, Ref. 118 also gives a review of some recent applications of the GLE, such as calculations of the atomic energy shift due to blackbody radiation [85], transport theory formulated for the center-of-mass of the electrons [84,121], elimination of runaway solutions for the radiating electron [93], dissipative quantum tunneling [90,91], and the calculation of the effect of charge fluctuations on current-voltage curves for small-capacitance tunnel junctions [122]. The relationship between the GLE model and the Landauer formula has also been explored recently [123].

The general question of the effect of a dissipative environment on localization has generated much interest due to the diversity of physical realizations, as well as to some advances in the theory over the last decade [53]. A specific problem that has been examined in most detail is the two-level system (the so-called spin-boson model) [99], in which an object describable by a single variable, say the generalized coordinate of a “particle”, moves in an effective potential of double-well shape. This model can be derived from an extended system by the truncation procedure [124]. If the bias energy (the energy difference between the two ground states in the two potential wells) is sufficiently small, compared to the tunneling matrix element energy, then coherent tunneling occurs between the two wells so that the particle coordinate is delocalized. The probability of finding the particle in either well at a given time oscillates sinusoidally between zero and one in the particular case of zero bias, with a frequency much smaller than that of the

classical oscillations of small amplitude in either well. This phenomenon of quantum phase coherence between the wave-function amplitudes for the two wells has well been observed for many microscopic systems, for example, the oscillations between the two sites of the nitrogen atom in an ammonia molecule (ammonia maser) and those between the two values of strangeness of a neutral K-meson. The two-level system in this regard is merely the simplest quantum system allowing constructive and destructive interference.

For the macroscopic quantum coherence (MQC) effect, dissipation has to be taken into account. It has been shown that in the case of sufficiently large Ohmic dissipation, the quantum phase coherence is destroyed in that a localization transition occurs resulting in the particle being confined to one well for all times [105]. Furthermore, at zero temperature, not only does localization occur for Ohmic dissipation but it also occurs in the sub-Ohmic case [99], whereas it was concluded that localization can never occur in the super-Ohmic case [03]. Generally speaking, sufficiently strong coupling of a quantum system to its environment destroys its phase coherence [100 – 102]. Deeper understanding of this phenomenon may be obtained, however, only by investigating realistic concrete models. Besides the spin-boson model, one such model is the IO model, which has the advantage over the former of being more tractable.

The mean square displacement of a quantum harmonic oscillator in a general heat bath in the framework of the IO model is studied in Ref. 125 (the body text of which constitutes Section 3 of this dissertation) to gain insight into the effects of dissipation on the localization of an oscillator. The degree of localization of the oscillator, as measured by its mean square displacement, is shown to increase with decreasing temperatures in an arbitrary physical heat bath as thermal fluctuations decrease with decreasing temperatures. For the Ohmic and blackbody radiation heat baths, either increase of oscillator frequency or of dissipation is found to lead to an enhancement of localization at any temperatures. This reduction in the width of the wave function of a harmonic oscillator by

contact with an environment is in accord with the theoretical prediction [77,115,116] and numerical calculations [126], also confirmed by experiments [107,108], that the quantum tunneling rate at zero temperature decreases with increasing dissipation in the absence of renormalization [90]. (For the blackbody radiation heat bath, on the other hand, the renormalization procedure is requisite and was found to lead to enhanced quantum tunneling rate instead [91].)

The reprints of Refs. 118 and 125 mentioned above form Sections 2 and 3, respectively, in Chapter II of this dissertation.

2. Correlation in the Langevin Theory of Brownian Motion*

I. Introduction

The motion of a "Brownian particle" [7] (an otherwise free particle in a dissipative environment) is described most elegantly by Langevin's stochastic classical differential equation [14]

$$m\ddot{x} + m\gamma\dot{x} = F(t) , \quad (1)$$

where m and x denote the mass and coordinate of the particle, respectively, and the dot denotes differentiation with respect to time. The force on the particle consists of the frictional (dissipative) term $-m\gamma\dot{x}$ and the random (fluctuation or noise) term $F(t)$.

Since the past motion does not appear in Eq. (1), one says there is no memory. In addition, the autocorrelation of the random force is a δ function and is also proportional to γ . The latter result is a manifestation of the fluctuation-dissipation relation.

*This section consists of the body text of Ref. 118, by X. L. Li, G. W. Ford, and R. F. O'Connell, with its abstract incorporated in Sec. 1 (Introduction to Chapter II) and its references merged into the overall bibliography. The authors very much appreciate the hospitality of the Dublin Institute for Advanced Studies and especially its Director, Professor J. T. Lewis, for hospitality extending over a decade of summers when part of this work was carried out. This research was partially supported by the National Science Foundation under Grant No. INT 920-4411 and by the U.S. Office of Naval Research under Grant No. N0001490-J-1124.

The question of the ensemble average of the product of the displacement and the random force was examined by Manoliu and Kittel in a paper in this journal [119]. In particular, they verified an assertion of Langevin that, for the case of Eq. (1),

$$\langle x(t)F(t) \rangle = 0 . \quad (2)$$

Equation (1) describes what is often referred to as the Ohmic (or Drude) model (no memory terms) of a classical heat bath. The question arises as to the correctness or otherwise of Eq. (2), when one considers more realistic models, since Eq. (1) is essentially a phenomenological model which has not been derived from microscopic considerations. Further, the calculations of Ref. 119 are confined to the case of high temperature. Thus we wish to consider the possible effect of extending the calculations of Ref. 119 to the quantum, arbitrary-temperature domain with inclusion of possible memory effects. In addition, we wish to go beyond Brownian motion by considering the effect of an external potential. The machinery required to do this is the generalized quantum Langevin equation (GLE). This equation will be discussed at length in the next section. We will then go on to apply our results to various situations and we show how the results of Manoliu and Kittel [119] get modified in the more general case. In particular, we also demonstrate that the results of Ref. 119 follow simply and elegantly from our general formalism. Finally, we present a discussion of our results.

However, before moving on to our specific problem, we would like to discuss its relevance to a broad range of investigations which incorporate dissipation and fluctuations as an essential element.

The study of fluctuation phenomena in science began in essence in 1827 with the observations of the Scottish botanist, Robert Brown [7]. It is interesting to note that these early observations are still a source of great interest and controversy [127]. An explanation of these results was first provided by Einstein [9] using a discrete time assumption.

An entirely new approach was later presented by Langevin [14] in the form of a stochastic differential equation. For a survey of this early work we refer to the treatise by Gardiner [65], but we would be remiss if we did not refer to the major contributions and extensions of the theory described in Refs. 15–17. It soon became apparent that a Langevin-type equation provides the framework for discussing fluctuation and dissipative phenomena over a wide spectrum of physical phenomena.

In general, there is an intimate connection between fluctuations and dissipation which is referred to as the fluctuation–dissipation (FD) theorem. For example, Nyquist [41] showed that the random fluctuations in voltage across a resistor measured by Johnson [42] are determined by its impedance. A general quantum formulation of the FD theorem appears in the celebrated paper of Callen and Welton [43]. This theorem is a key ingredient of the pioneering work of Kubo [28,39] on linear response theory in nonequilibrium statistical mechanics. Correlations of the type discussed in the present paper are widely used in the work of Kubo and others. Another major advance is contained in the work of Mori [64], who showed that a microscopic equation of motion can generally be transformed into the form of a GLE.

Over the past ten years, two of us (G.W.F. and R.F.O.) have collaborated extensively with Lewis on problems involving the GLE. In Ref. 82 we gave a detailed discussion of this equation and we discussed various models of a heat bath which have appeared in the literature. The particular case of a blackbody radiation heat bath was discussed at length [82,83] for the purpose of calculating atomic energy shifts due to blackbody radiation [85]. Transport theory was also discussed [84] and, in fact, Hu and O’Connell have shown that a many-body Hamiltonian problem may be reformulated in terms of a GLE for the center-of-mass of the electrons [121], which led them to an expression for the conductivity which is actually simpler than that obtained using the Kubo approach. In addition, we note that G.W.F. and R.F.O. returned to the problem of a blackbody

radiation heat bath to obtain an improved equation for the radiating electron [93]; this equation, in contrast to the Abraham–Lorentz equation, is second order, it does not display runaway solutions and it leads to a modification of the familiar Larmor formula [93].

Modern lithographic methods have led to a burgeoning of interest in mesoscopic systems which, by their nature, are more sensitive to the dissipative effects caused by their environment. In particular, quantum tunneling in a variety of systems is affected by dissipation, a subject which was discussed in the pioneering paper of Caldeira and Leggett [77]. The starting point of the latter authors and most others [112] is a Lagrangian which permits use of path integral, instanton, and functional integral methods. By contrast, our starting point is a Hamiltonian which is used to derive a GLE. In particular, this enabled us to develop a GLE approach to dissipative quantum tunneling [90]. The Langevin approach has also been used by Cleland *et al.* and by Hu and O’Connell [122] to calculate the effect of charge fluctuations, arising from the environment, on current-voltage curves for small-capacitance tunnel junctions.

Finally, we note that Brownian motion is being interpreted in a new light by investigators in the relatively new field of fractals; the path of the microscopic particles observed by Brown is referred to as a Brownian fractal curve [23].

II. Generalized Quantum Langevin Equation

In recent years, there has been widespread interest in dissipative problems arising in a variety of areas in physics. As it turns out, solutions of many of these problems are encompassed by a generalization of Eq. (1) to encompass quantum, memory, and non-Markovian effects, as well as arbitrary temperature and the presence of an external potential $V(x)$. We refer to this as the GLE

$$m\ddot{x} + \int_{-\infty}^t dt' \mu(t-t') \dot{x}(t') + V'(x) = F(t) , \quad (3)$$

where $V'(x) = dV(x)/dx$ is the negative of the time-independent external force and $\mu(t)$ is the so-called memory function.

A detailed discussion of Eq. (3) appears in Ref. 82. In particular, it was pointed out that the GLE corresponds to a macroscopic description of a quantum system interacting with a quantum-mechanical heat bath and that this description can be precisely formulated, using such general principles as causality and the second law of thermodynamics. We also stressed that this is a model-independent description. However, the GLE can be realized with a simple and convenient model, viz., the independent-oscillator (IO) model. The Hamiltonian of the IO system is

$$H = \frac{p^2}{2m} + V(x) + \sum_j \left[\frac{p_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 (q_j - x)^2 \right]. \quad (4)$$

Here m is the mass of the quantum particle while m_j and ω_j refer to the mass and frequency, respectively, of heat-bath oscillator j . In addition, x and p are the coordinate and momentum operators, respectively, for the quantum particle, and q_j and p_j are the corresponding quantities for the heat-bath oscillators. Use of the Heisenberg equations of motion leads to the GLE, Eq. (3), describing the time development of the particle motion, with

$$\mu(t) = \sum_j m_j \omega_j^2 \cos(\omega_j t) \theta(t), \quad (5)$$

where $\theta(t)$ is the Heaviside step function. Also

$$F(t) = \sum_j m_j \omega_j^2 q_j^h(t), \quad (6)$$

where $q_j^h(t)$ denotes the general solution of the homogeneous equation for the heat-bath oscillators (corresponding to no interaction). These results were used to obtain the (model-independent) result for the (symmetric) autocorrelation of $F(t)$, viz.,

$$\frac{1}{2} \langle F(t)F(t') + F(t')F(t) \rangle = \frac{1}{\pi} \int_0^\infty d\omega \operatorname{Re} [\tilde{\mu}(\omega + i0^+)] \hbar \omega \coth\left(\frac{\hbar \omega}{2kT}\right) \cos[\omega(t - t')], \quad (7)$$

where $\tilde{\mu}(\omega)$ is the Fourier transform of the memory function $\mu(t)$. This type of equation is referred to by Kubo [28] as the second fluctuation–dissipation theorem and we note that it can be written down explicitly once the GLE is obtained. On the other hand, the first fluctuation–dissipation theorem is an equation involving the autocorrelation of $x(t)$ and its explicit evaluation requires a knowledge of the generalized susceptibility $\alpha(\omega)$ (to be defined below) which is equivalent to knowing the solution to the GLE. This solution is readily obtained when $V(x) = 0$, corresponding to the original Brownian-motion problem. As shown by Ford, Lewis, and O’Connell [83,84], a solution is also possible in the case of an oscillator. Taking $V(x) = (1/2)m\omega_0^2 x^2$, these authors obtained [see Eqs. (1)–(3) of Ref. 83]

$$\tilde{x}(\omega) = \alpha(\omega) \tilde{F}(\omega) , \quad (8)$$

where

$$\alpha(\omega) = \left[-m\omega^2 + m\omega_0^2 - i\omega\tilde{\mu}(\omega) \right]^{-1} \quad (9)$$

and the superposed tilde is used to denote the Fourier transform. Thus, $\tilde{x}(\omega)$ is the Fourier transform of the operator $x(t)$

$$\tilde{x}(\omega) = \int_{-\infty}^{\infty} dt x(t) e^{i\omega t} . \quad (10)$$

Also, since Eq. (5) implies that $\mu(t)$ is 0 for negative t , we have

$$\tilde{\mu}(\omega) = \int_0^{\infty} dt \mu(t) e^{i\omega t} , \quad \text{Im } \omega > 0 . \quad (11)$$

Thus $\tilde{\mu}(\omega)$ is analytic in the upper half-plane, $\text{Im } \omega > 0$.

We have now all the tools we need to calculate various correlation functions. Before doing so, it is convenient to rewrite Eq. (7) in the form

$$C_{FF}(\tau) \equiv \frac{1}{2} \langle F(t)F(t') + F(t')F(t) \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \tilde{C}_{FF}(\omega) e^{-i\omega\tau}, \quad (12)$$

where $\tau = t - t'$ and where

$$\tilde{C}_{FF}(\omega) = \text{Re} \left[\tilde{\mu}(\omega + i0^+) \right] \hbar \omega \coth(\hbar \omega / 2kT). \quad (13)$$

In deriving this result we have used the fact that the integrand on the right-hand side of Eq. (7) is an even function of ω . Next, using Eqs. (8) and (12), it is straightforward to prove that

$$C_{xx}(\tau) \equiv \frac{1}{2} \langle x(t)x(t') + x(t')x(t) \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \tilde{C}_{xx}(\omega) e^{-i\omega\tau}, \quad (14)$$

where

$$\tilde{C}_{xx}(\omega) = |\alpha(\omega)|^2 \tilde{C}_{FF}(\omega) = \hbar \text{Im} \alpha(\omega) \coth(\hbar \omega / 2kT), \quad (15)$$

where the second equality in Eq. (15) follows from use of the relation

$$\text{Im} \alpha(\omega) = \omega |\alpha(\omega)|^2 \text{Re} \tilde{\mu}(\omega), \quad (16)$$

which, in turn, follows directly from Eq. (9). We note that Eqs. (14) and (15) are nothing more than the fluctuation–dissipation theorem of the first kind [28].

In a similar manner, we obtain, for the ensemble average of the product of the displacement and random force, the quantity of interest to Manoliu and Kittel [119], the result

$$C_{XF}(\tau) \equiv \frac{1}{2} \langle x(t)F(t') + F(t')x(t) \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \tilde{C}_{XF}(\omega) e^{-i\omega\tau}, \quad (17)$$

where

$$\tilde{C}_{XF}(\omega) = \alpha(\omega) \tilde{C}_{FF}(\omega) = \alpha(\omega) \text{Re} \tilde{\mu}(\omega) \hbar \omega \coth(\hbar \omega / 2kT). \quad (18)$$

Equations (17) and (18) provide a general expression for the desired ensemble average of the product of the displacement and the random force. Since it is generally convenient to evaluate the integral appearing in Eq. (17) by use of contour integration, it is useful to recall that ω has a positive imaginary part. Thus in carrying out contour integrations, it should be noted that the contour will be an amount 0^+ above the real axis or, in other words, it will go from $-\infty + i\varepsilon$ to $\infty + i\varepsilon$ where $\varepsilon = 0^+$. In this context, we note that $\alpha(\omega)$ is an analytic function in the upper half-plane (UHP). Finally, $\coth(\hbar\omega/2kT)$ has simple poles at $\omega = i\omega_n$ (with $n = 0, \pm 1, \pm 2, \dots$), where

$$\omega_n = (2\pi kT/\hbar)n \quad (19)$$

are the Matsubara frequencies [128,129]. Also, the residue of each of these poles is $2kT/\hbar$.

III. Results For The Position-Force Correlation

A. Classical Brownian motion in an Ohmic heat bath

The original Brownian motion problem is described by Eq. (1), corresponding to a free particle ($\omega_0 = 0$) in an Ohmic heat bath [$\text{Re}\tilde{\mu}(\omega) = m\gamma$ or $\mu(t) = m\gamma\delta(t)$, which implies no memory effects] and also $kT \gg \hbar\gamma$ (absence of quantum effects). This corresponds to the case considered in Ref. 119. Then, using Eq. (18), we see that Eq. (17) reduces to

$$C_{XF}(\tau) = kT \frac{m\gamma}{\pi} \int_{-\infty}^{\infty} d\omega \alpha(\omega) e^{-i\omega\tau} = 2m\gamma kTG(\tau), \quad (20)$$

where $G(\tau)$ is, by definition, the inverse Fourier transform of $\alpha(\omega)$. [This is the only exception to our convention of denoting the Fourier transform of any function, $A(t)$ say, by $\tilde{A}(\omega)$. The reason for this exception is to conform to commonly accepted practice in the literature.] In the above limits ($\omega_0 = 0$ and $\text{Re}\tilde{\mu}(\omega) = m\gamma$), we also see, from Eq. (9), that $\alpha(\omega) = [-m\omega(\omega + i\gamma)]^{-1}$.

We now turn to the evaluation of the integral in Eq. (20). For $\tau < 0$, we complete the contour in the UHP. But, since $\alpha(\omega)$ is analytic in the UHP, it follows that

$$C_{XF}(\tau) = 0 \quad \text{if } \tau < 0. \quad (21)$$

In other words, the correlation between the position x at time t and the fluctuation F at a later time t' is zero. This is in conformity with our physical intuition that there is no effect before a cause (causality principle).

In the case where $\tau > 0$, we complete the contour in the lower half-plane (LHP). Since $\alpha(\omega)$ has poles at $\omega = 0$ and $\omega = -i\gamma$, it follows from Eq. (20) that

$$C_{XF}(\tau) = 2kT(1 - e^{-\gamma\tau}) \quad \text{if } \tau > 0. \quad (22)$$

In particular, we note that $C_{XF}(0) = 0$ and also that $C_{XF}(\tau) \rightarrow 0$ as $\gamma \rightarrow 0$. Also, Eq. (22) corresponds to the result obtained in Ref. 119 [see their Eqs. (7) and (19)]. Thus, if the force is applied at a time t' there is a correlation between it and the position of the particle at a later time t . Another way of seeing this is to note that if we take the inverse Fourier transform of Eq. (8) then, by the Fourier convolution theorem,

$$x(t) = \int_{-\infty}^t dt' G(t-t') F(t'), \quad (23)$$

where $G(t)$, the retarded Green's function, is the inverse Fourier transform of $\alpha(\omega)$, i.e.,

$$G(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \alpha(\omega) e^{-i\omega t}, \quad (24)$$

and it is clear from Eq. (24), and the fact that $\alpha(\omega)$ has no poles in the UHP, that $G(t)$ is zero for $t < 0$. We see from Eq. (23) that $x(t)$ is determined by the force at all previous times from $-\infty$ to t , which explains the correlation between $x(t)$ and $F(t')$ for the case $t > t'$ (i. e., $\tau > 0$) since, in this case, $x(t)$ contains a contribution from $F(t')$. Thus,

even in this simple case, there is a manifestation of “memory” in the relation between the displacement and the fluctuation force, as is made manifest in Eq. (23).

B. Brownian motion at arbitrary temperature in an Ohmic heat bath

As in subsection III A, we take $\text{Re } \tilde{\mu}(\omega) = m\gamma$ and $\omega_0 = 0$ so that Eq. (17) becomes

$$\begin{aligned} C_{XF}(\tau) &= \frac{m\gamma}{2\pi} \int_{-\infty}^{\infty} d\omega \hbar\omega \alpha(\omega) \coth(\hbar\omega/2kT) e^{-i\omega\tau} \\ &= -\frac{\hbar\gamma}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{1}{\omega + i\gamma} \coth(\hbar\omega/2kT) e^{-i\omega\tau}. \end{aligned} \quad (25)$$

For $\tau < 0$, in contrast to subsection III A, this quantity is no longer zero because of the poles of $\coth(\hbar\omega/2kT)$ in the UHP at $\omega = i\omega_n$ ($n = 1, 2, \dots$). Thus

$$C_{XF}(\tau) = -2kT\gamma \sum_{n=1}^{\infty} \frac{1}{\omega_n + \gamma} e^{-\omega_n |\tau|} \quad \text{if } \tau < 0, \quad (26)$$

where ω_n is given by Eq. (19). It is clear that $C_{XF}(\tau) \rightarrow 0$ in the high-temperature limit and also in the limit $\gamma \rightarrow 0$.

The question now arises as to why, in the case $\tau < 0$, we get a nonzero result here, as distinct from subsection III A. The answer is that in the latter case, it is clear, using Eqs. (12) and (13), that $C_{FF}(\tau)$, the autocorrelation of the random force, is equal to $2m\gamma kT\delta(\tau)$, i.e., we are dealing with “white noise”. On the other hand, $C_{FF}(\tau)$ is not proportional to a δ function in this subsection. [See the discussion after Eq. (2.11) in Ref. 82 where, in particular, we point out that “... although there is no memory, the quantum-mechanical process is not Markovian in the customary sense of the term”.] As a result, for $t < t'$, we deduce that $x(t)$ [which according to Eq. (23) contains contributions from $F(t'')$ for all values of $t'' < t$] can be correlated with $F(t')$, the random force at a later time.

Considering now the case $\tau > 0$, our contour integral is in the LHP and encloses poles at $\omega = -i\omega_n$ ($n = 0, 1, 2, \dots$) and at $\omega = -i\gamma$. Thus, from (25) and the fact that $\coth(ix) = -i \cot(x)$, we obtain

$$\begin{aligned} C_{XF}(\tau) &= -\hbar\gamma \cot\left(\frac{\hbar\gamma}{2kT}\right) e^{-\gamma\tau} + 2kT \left(1 - \gamma \sum_{n=1}^{\infty} \frac{1}{\omega_n - \gamma} e^{-\omega_n\tau}\right) \\ &= 2kT\gamma \left[\sum_{n=0}^{\infty} \frac{1}{\omega_n - \gamma} (e^{-\gamma\tau} - e^{-\omega_n\tau}) - \sum_{n=1}^{\infty} \frac{1}{\omega_n + \gamma} e^{-\gamma\tau} \right] \quad \text{if } \tau > 0, \end{aligned} \quad (27)$$

where ω_n is given by Eq. (19). In the high-temperature limit, it is clear that Eq. (27) reduces to Eq. (22). Finally, we note, from the $\tau \rightarrow 0$ limits of Eqs. (26) and (27), that $C_{XF}(\tau)$ approaches the same logarithmic divergence from both sides of $\tau = 0$.

C. Brownian motion of a charged particle in a blackbody radiation heat bath

The motion of a charged oscillator (with charge e and natural frequency ω_0) in a blackbody radiation heat bath was discussed extensively in Refs. 82, 83, and 84. We take the limit $\omega_0 = 0$ of these results for the Brownian motion problem (which also implies that the corresponding “ γ ” is zero since $\gamma = \omega_0^2 \tau_e$ in this case) [82,83] to get, in the large-cutoff limit,

$$\alpha(\omega) = -(1 - i\omega\tau_e)/M\omega^2, \quad (28)$$

and

$$\text{Re } \tilde{\mu}(\omega) = M\tau_e^{-1}\omega^2 / (\omega^2 + \tau_e^{-2}), \quad (29)$$

where M is the renormalized (physically observable) mass of the charged particle and $\tau_e \equiv 2e^2/3Mc^3 = 6.27 \times 10^{-24}$ s, for the electron. Therefore

$$\alpha(\omega) \text{Re } \tilde{\mu}(\omega) = i / (\omega - i\tau_e^{-1}). \quad (30)$$

We will now combine this result with Eqs. (17) and (18). We will also consider only the high-temperature limit in order to separate quantum effects from memory effects which clearly arise from the frequency-dependence of $\text{Re } \tilde{\mu}(\omega)$. Thus

$$C_{XF}(\tau) = \frac{ikT}{\pi} \int_{-\infty}^{\infty} d\omega \frac{1}{\omega - i\tau_e^{-1}} e^{-i\omega\tau} . \quad (31)$$

Since the integrand has only one pole at $\omega = i\tau_e^{-1}$, it follows that

$$C_{XF}(\tau) = -2kT \exp(-|\tau|/\tau_e) \quad \text{if } \tau < 0 . \quad (32)$$

In addition, it would appear from Eq. (31) that $C_{XF}(\tau) = 0$ if $\tau > 0$. However, this is not so. The reason is that our expression for $\alpha(\omega)$ given in Eq. (28) incorporates the large-cutoff limit of quantum electrodynamics (see the discussion in Refs. 83 and 84). For most applications (such as the $\tau < 0$ calculation which we have just carried out) this is permissible. However, there are other situations (such as the $\tau > 0$ calculation) for which the large-cutoff limit should not be taken until the end of the calculation. Thus, more generally, when reduced to its essentials, the expression for $\alpha(\omega)$ given in Eq. (28) should be multiplied by the factor $i\Omega'/(\omega + i\Omega')$ and then one lets $\Omega' \rightarrow \infty$ at the end of the calculation. [The denominator factor $(\omega + i\Omega')$ first appears in Eq. (19) of Ref. 83 and we refer to the discussion following this equation, and also to Ref. 84, for further details.] This factor does not affect the calculation for $\tau < 0$ where we are only concerned with poles in the UHP. However, for $\tau > 0$, we have now got a pole at $\omega = -i\Omega'$ in the LHP so, as a consequence,

$$C_{XF}(\tau) = -2kT \exp(-\Omega'\tau) \quad \text{if } \tau > 0 . \quad (33)$$

For all nonzero positive values of τ this expression gives 0 in the limit $\Omega' \rightarrow \infty$ but if we let $\tau \rightarrow 0$ prior to letting $\Omega' \rightarrow \infty$ then we get $C_{XF}(0) = -2kT$, in agreement with Eq. (32). In other words, the correlation function is also continuous at $\tau = 0$ provided that

we go to the large-cutoff limit by letting Ω' be very large but not infinite. The nonzero result here should be contrasted with the zero result given by Eqs. (21) and (22) in the limit $\gamma \rightarrow 0$. This is a manifestation of memory effects. It is surprisingly large and it reflects the fact that the random force autocorrelation function is no longer a δ function.

D. Classical oscillator in an Ohmic heat bath

Here, we are going beyond Brownian motion to consider the effect of a harmonic confining potential. The equation of motion in this case is

$$m\ddot{x} + m\gamma\dot{x} + m\omega_0^2 x = F(t) . \quad (34)$$

Thus $\text{Re} \tilde{\mu}(\omega) = m\gamma$, as in case A but now,

$$\alpha(\omega) = \left[-m(\omega^2 + i\gamma\omega - \omega_0^2) \right]^{-1} . \quad (35)$$

It follows that $C_{XF}(\tau)$ is still given by Eq. (20) but now

$$G(\tau) = -\frac{1}{2\pi m} \int_{-\infty}^{\infty} d\omega \frac{1}{(\omega - \omega_a)(\omega - \omega_b)} e^{-i\omega\tau} , \quad (36)$$

where

$$\omega_{a,b} = \mp\omega_1 - i(\gamma/2) \quad (37)$$

and

$$\omega_1 = \left\{ \omega_0^2 - (\gamma/2)^2 \right\}^{1/2} . \quad (38)$$

Also, we are assuming $\omega_0 > (\gamma/2)$ but we will consider the reverse case below. Thus, since both poles of the integrand lie in the LHP, it follows immediately that

$$C_{XF}(\tau) = 0 \quad \text{if } \tau < 0 . \quad (39)$$

For $\tau > 0$, we obtain

$$G(\tau) = \frac{i}{m} \left(\frac{e^{-i\omega_a\tau}}{\omega_a - \omega_b} + \frac{e^{-i\omega_b\tau}}{\omega_b - \omega_a} \right) = \frac{1}{m\omega_1} \sin(\omega_1\tau) e^{-(\gamma/2)\tau} \quad \text{if } \tau > 0. \quad (40)$$

Thus, using Eq. (20), we obtain

$$C_{XF}(\tau) = (2\gamma kT/\omega_1) \sin(\omega_1\tau) e^{-(\gamma/2)\tau} \quad \text{if } \tau > 0 \text{ and } \omega_0 > (\gamma/2). \quad (41)$$

It is clear that $C_{XF}(\tau) \rightarrow 0$ as $\gamma \rightarrow 0$ and also $C_{XF}(0) = 0$.

In the case where $\omega_0 < (\gamma/2)$, we can still use Eq. (36) except that now

$$\omega_{a,b} = -i[(\gamma/2) \pm \omega_2], \quad (42)$$

where

$$\omega_2 = [(\gamma/2)^2 - \omega_0^2]^{1/2}. \quad (43)$$

As before, both poles lie in the LHP. Thus Eq. (39) again holds but now Eq. (41) is replaced by

$$C_{XF}(\tau) = (\gamma kT/\omega_2) e^{-(\gamma/2)\tau} [e^{\omega_2\tau} - e^{-\omega_2\tau}] \quad \text{if } \tau > 0 \text{ and } \omega_0 < (\gamma/2). \quad (44)$$

In the limit $\omega_0 \ll (\gamma/2)$, we now see that $\omega_2 = (\gamma/2)[1 - 2(\omega_0/\gamma)^2 + \dots]$ and hence

$$C_{XF}(\tau) \cong 2kT(1 - e^{-\gamma\tau}) \left\{ 1 + (\omega_0/\gamma)^2 \left[2 - \gamma\tau(1 + e^{-\gamma\tau}) / (1 - e^{-\gamma\tau}) \right] \right\} \quad \text{if } \tau > 0. \quad (45)$$

In the limit $\omega_0 \rightarrow 0$, we see that this result reduces to that given in Eq. (22). Further, it shows that the effect of the harmonic potential is to decrease the correlation between the displacement and the random force.

IV. Conclusions

We have considered Brownian motion in a very general heat bath by means of a GLE. We also presented a solution to this equation (and also to the more general equation describing the case of a harmonically bound particle in a heat bath). Next, these results are used to calculate the correlation between the displacement $x(t)$ and the random force $F(t)$ and it is shown that the classical limit of these results reproduce, in a simple and elegant manner, the results of Ref. 119. Particular emphasis was placed on “memory effects”, as exemplified by consideration of the blackbody radiation heat bath.

3. Dissipative Effects on the Mean Square Displacement of an Oscillator*

I. Introduction

Dissipative effects are ubiquitous in many areas of physics. In some previous publications [82 – 84] we argued the merits of treating an exactly solvable model of a heat bath, which we referred to as the IO model [82]. In particular, this model can be shown to describe many kinds of dissipative environments, such as Ohmic heat baths or the physically important case of a blackbody radiation heat bath [82].

In order to gain further insight into the nature of the IO model, we are motivated to examine in detail the effect of dissipation on the mean square displacement or, equivalently, the equal-time position autocorrelation function. In particular, such a quantity may be used to calculate the effect of dissipation on the localization of an oscillator. Some investigations have already been carried out for the case of an Ohmic heat bath [77]. Our purpose here is to expand these investigations but, more important, to extend these considerations to the case of a blackbody radiation heat bath.

*This section consists of the body text of Ref. 125, by X. L. Li, G. W. Ford, and R. F. O’Connell, with its abstract incorporated in Sec. 1 (Introduction to Chapter II) and its references merged into the overall bibliography. This research was partially supported by the U.S. Office of Naval Research under Contract No. N00014-90-J-1124 and by the National Science Foundation, Grant No. INT-890-2519. One of us (RFO’C) would like to thank Dr. Peter Knight for encouraging him to do this problem some years ago.

A powerful tool for solving the problem of the interaction of a quantum system with a heat bath is the generalized quantum Langevin equation, which, for a particle of mass m in a harmonic potential well with spring constant K , takes the form [82 – 84]

$$m\ddot{x} + \int_{-\infty}^t dt' \mu(t-t')\dot{x}(t') + Kx = F(t) . \quad (1.1)$$

This is an equation for the time-dependent Heisenberg operator $x(t)$. The coupling with the heat bath corresponds to two terms: an operator-valued random force $F(t)$ with mean zero, and a mean force characterized by a memory function $\mu(t)$. Forming the Fourier transform of (1.1), we obtain

$$\tilde{x}(\omega) = \alpha(\omega) \tilde{F}(\omega) , \quad (1.2)$$

where the superposed tilde denotes the Fourier transform, and $\alpha(\omega)$ is the generalized susceptibility (a c-number) given by

$$\alpha(\omega) = [-m\omega^2 + K - i\omega\tilde{\mu}(\omega)]^{-1} , \quad (1.3)$$

where

$$\tilde{\mu}(\omega) = \int_0^{\infty} dt \mu(t) e^{i\omega t} , \quad \text{Im } \omega > 0 , \quad (1.4)$$

called the spectral distribution, is the Fourier transform of the memory function. It is analytic in the upper half of the ω plane and its real part is positive on the real axis [82]. Such functions are termed positive functions. It can be shown that $-i\omega\alpha(\omega)$ is also a positive function provided that m and K are positive [82 – 84]. It follows that

$$\text{Im } \alpha(\omega) > 0 \quad \text{for } \omega > 0 . \quad (1.5)$$

The generalized susceptibility plays an important role in determining the dynamics of the system. On applying the fluctuation–dissipation theorem, we immediately obtain [77,88]

$$\langle x^2 \rangle = \frac{\hbar}{\pi} \int_0^\infty d\omega \coth\left(\frac{\hbar\omega}{2kT}\right) \text{Im}[\alpha(\omega + i0^+)] . \quad (1.6)$$

Since the factor $\coth(\hbar\omega/2kT)$ in the integrand of (1.6) is a monotonically increasing function of T , it follows, by (1.5), that $\langle x^2 \rangle$ is also a monotonically increasing function of T , i.e.,

$$\frac{\partial}{\partial T} \langle x^2 \rangle > 0 . \quad (1.7)$$

In other words, as we might expect, in the case of an arbitrary spectral distribution, *higher temperatures favor delocalization*.

In sections II and III, we shall calculate in detail, using (1.6), the mean square oscillator displacement and its derivatives for both Ohmic and blackbody radiation heat baths, at zero and nonzero temperatures. In section IV, we present our conclusions.

II. Ohmic Heat Bath

This is the simplest type of heat bath with $\tilde{\mu}(\omega) = m\gamma$, a constant independent of the frequency ω . The corresponding generalized susceptibility, by (1.3), is

$$\alpha(\omega) = \frac{1}{m(\omega_0^2 - \omega^2 - i\gamma\omega)} , \quad (2.1)$$

where

$$\omega_0^2 = \frac{K}{m} . \quad (2.2)$$

Then

$$\begin{aligned}
\text{Im } \alpha(\omega) &= \frac{\gamma \omega}{m \left[(\omega^2 - \omega_0^2)^2 + \gamma^2 \omega^2 \right]} \\
&= \frac{\omega}{2m} \text{Im} \left[\frac{1}{\sqrt{\omega_0^2 - \gamma^2/4}} \left(\frac{1}{\omega^2 + \omega_2^2} - \frac{1}{\omega^2 + \omega_1^2} \right) \right], \quad (2.3)
\end{aligned}$$

where $\omega_{1,2} = \gamma/2 \pm i\sqrt{\omega_0^2 - \gamma^2/4}$.

At zero temperature ($T = 0$ K), $\coth(\hbar\omega/2kT) = 1$. Inserting this and (2.3) in (1.6), we obtain the mean square oscillator displacement at zero temperature [77]

$$\begin{aligned}
\langle x^2 \rangle|_{T=0} &= \frac{\hbar}{\pi} \int_0^\infty d\omega \text{Im}[\alpha(\omega)] = \frac{\hbar}{2\pi m} \text{Im} \left[\frac{1}{\sqrt{\omega_0^2 - \gamma^2/4}} \ln \left(\frac{\omega_1}{\omega_2} \right) \right] \\
&= \frac{\hbar}{\pi m \sqrt{\omega_0^2 - \gamma^2/4}} \tan^{-1} \left(\frac{2}{\gamma} \sqrt{\omega_0^2 - \gamma^2/4} \right) \\
&= \frac{\hbar}{\pi m \sqrt{\omega_0^2 - \gamma^2/4}} \sin^{-1} \left(\frac{1}{\omega_0} \sqrt{\omega_0^2 - \gamma^2/4} \right) \quad \text{if } \omega_0 > \frac{1}{2}\gamma
\end{aligned}$$

and

$$\langle x^2 \rangle|_{T=0} = \frac{\hbar}{2\pi m \sqrt{\gamma^2/4 - \omega_0^2}} \ln \left(\frac{\gamma/2 + \sqrt{\gamma^2/4 - \omega_0^2}}{\gamma/2 - \sqrt{\gamma^2/4 - \omega_0^2}} \right) \quad \text{if } \omega_0 < \frac{1}{2}\gamma. \quad (2.4)$$

From (2.4) we see that for $\omega_0 \ll (\gamma/2)$ this function reduces to $2\hbar/\pi m \gamma \ln(\gamma/\omega_0)$, for $\omega_0 \gg (\gamma/2)$ it reduces to $\hbar/2m\omega_0$, and for $\omega_0 = (\gamma/2)$ it equals $\hbar/\pi m \omega_0 = 2\hbar/\pi m \gamma$. These results already appear in the work of Ref. 77 (p. 437). Our purpose here is to use them to investigate the detailed behavior of the mean square displacement on the parameters γ and K and eventually compare them with the corresponding results in the case of a blackbody radiation heat bath.

It is then straightforward to check that

$$\frac{\partial}{\partial \gamma} \langle x^2 \rangle = \begin{cases} \frac{\hbar \gamma}{4\pi m (\omega_0^2 - \gamma^2/4)^{3/2}} \left[\tan^{-1} \left(\frac{2}{\gamma} \sqrt{\omega_0^2 - \gamma^2/4} \right) - \frac{2}{\gamma} \sqrt{\omega_0^2 - \gamma^2/4} \right] & \text{if } \omega_0 > \frac{1}{2} \gamma, \\ \frac{\hbar \gamma}{8\pi m (\gamma^2/4 - \omega_0^2)^{3/2}} \left[\frac{4}{\gamma} \sqrt{\gamma^2/4 - \omega_0^2} - \ln \left(\frac{\gamma/2 + \sqrt{\gamma^2/4 - \omega_0^2}}{\gamma/2 - \sqrt{\gamma^2/4 - \omega_0^2}} \right) \right] & \text{if } \omega_0 < \frac{1}{2} \gamma, \end{cases} \quad (2.5)$$

and that

$$\frac{\partial}{\partial K} \langle x^2 \rangle = \begin{cases} \frac{\hbar}{2\pi m^2 (\omega_0^2 - \gamma^2/4)^{3/2}} \left[\frac{\gamma}{2\omega_0^2} \sqrt{\omega_0^2 - \gamma^2/4} - \tan^{-1} \left(\frac{2}{\gamma} \sqrt{\omega_0^2 - \gamma^2/4} \right) \right] & \text{if } \omega_0 > \frac{1}{2} \gamma, \\ \frac{\hbar}{4\pi m^2 (\gamma^2/4 - \omega_0^2)^{3/2}} \left[\ln \left(\frac{\gamma/2 + \sqrt{\gamma^2/4 - \omega_0^2}}{\gamma/2 - \sqrt{\gamma^2/4 - \omega_0^2}} \right) - \frac{\gamma}{\omega_0^2} \sqrt{\gamma^2/4 - \omega_0^2} \right] & \text{if } \omega_0 < \frac{1}{2} \gamma. \end{cases} \quad (2.6)$$

Both derivatives may be shown to be negative by use of the inequalities: $\tan^{-1} x < x$ ($x > 0$) and $(1/2) \ln[(1+x)/(1-x)] > x$ ($0 < x < 1$) in (2.5); $\tan^{-1} x > x/(1+x^2)$ ($x > 0$) and $(1/2) \ln[(1+x)/(1-x)] < x/(1-x^2)$ ($0 < x < 1$) in (2.6), respectively. Thus we conclude that, at zero temperature, localization becomes enhanced due to increasing of γ (i.e., damping) or K (i.e., binding).

Next we consider the case of nonzero temperature. Since

$$\coth(\hbar\omega/2kT) = 1 + \frac{2}{\exp(\hbar\omega/kT) - 1}, \quad (2.7)$$

denoting the temperature-dependent part of $\langle x^2 \rangle$ as $\Delta \langle x^2 \rangle$, we have

$$\begin{aligned}\Delta\langle x^2 \rangle &\equiv \langle x^2 \rangle - \langle x^2 \rangle|_{T=0} \\ &= \frac{2\hbar}{\pi} \int_0^\infty d\omega \frac{1}{\exp(\hbar\omega/kT) - 1} \text{Im}[\alpha(\omega)] .\end{aligned}\quad (2.8)$$

Using (2.3), this becomes

$$\Delta\langle x^2 \rangle = \frac{\hbar}{2\pi m} \text{Im} \left\{ \frac{1}{\sqrt{\omega_0^2 - \gamma^2/4}} \left[\ln\left(\frac{z_2}{z_1}\right) + \psi(z_1) - \psi(z_2) + \frac{1}{2z_1} - \frac{1}{2z_2} \right] \right\}, \quad (2.9)$$

where

$$z_{1,2} \equiv \frac{\hbar}{2\pi kT} \omega_{1,2}, \quad (2.10)$$

and we have used the formula

$$2 \int_0^\infty \frac{t dt}{[\exp(2\pi t) - 1](t^2 + z^2)} = \ln z - \psi(z) - \frac{1}{2z} \quad \left(|\arg z| < \frac{1}{2}\pi \right), \quad (2.11)$$

where $\psi(z) = d \ln \Gamma(z)/dz$ is the logarithmic derivative of the gamma function [130].

Hence

$$\begin{aligned}\langle x^2 \rangle &= \langle x^2 \rangle|_{T=0} + \Delta\langle x^2 \rangle \\ &= \frac{\hbar}{2\pi m} \text{Im} \left[\frac{1}{\sqrt{\omega_0^2 - \gamma^2/4}} \left(\psi(z_1) - \psi(z_2) + \frac{1}{2z_1} - \frac{1}{2z_2} \right) \right].\end{aligned}\quad (2.12)$$

In the high-temperature limit, $z_{1,2} \ll 1$, this expression becomes

$$\langle x^2 \rangle = \frac{kT}{m\omega_0^2} + \frac{\hbar^2}{12mkT} - \frac{\hbar^3 \gamma \zeta(3)}{4\pi^3 m (kT)^2} + \dots, \quad (2.13)$$

where $\zeta(3) = 1.202\dots$ [$\zeta(n)$ is the Riemann zeta function]. The leading term in (2.13) is the familiar classical result.

In the low-temperature limit, $z_{1,2} \gg 1$, (2.12) becomes

$$\langle x^2 \rangle = \frac{\hbar}{\pi m \sqrt{\omega_0^2 - \gamma^2/4}} \tan^{-1} \left(\frac{2}{\gamma} \sqrt{\omega_0^2 - \gamma^2/4} \right) + \frac{\pi \gamma (kT)^2}{3 \hbar m \omega_0^4} + \dots \quad (2.14)$$

Taking the derivatives of (2.12), one can readily show that

$$\frac{\partial}{\partial \gamma} \langle x^2 \rangle = -\frac{\hbar}{4 \pi m (\omega_0^2 - \gamma^2/4)} \operatorname{Re} \left\{ \frac{z_2 + z_1}{z_2 - z_1} [\psi(z_1) - \psi(z_2)] + z_1 \psi'(z_1) + z_2 \psi'(z_2) \right\}, \quad (2.15)$$

and that

$$\begin{aligned} \frac{\partial}{\partial K} \langle x^2 \rangle &= -\frac{\hbar^2}{4 \pi^2 m^2 kT (\omega_0^2 - \gamma^2/4)} \\ &\times \operatorname{Re} \left\{ \frac{\psi(z_1) - \psi(z_2)}{z_1 - z_2} - \frac{1}{2} [\psi'(z_1) + \psi'(z_2)] + \frac{1}{4} \left(\frac{1}{z_1} - \frac{1}{z_2} \right)^2 \right\}. \end{aligned} \quad (2.16)$$

By means of the partial-fractional expansion of $\psi(z)$,

$$\psi(z) = -C - \frac{1}{z} + \sum_{n=1}^{\infty} \frac{z}{n(n+z)} \quad (z \neq 0, -1, -2, -3, \dots), \quad (2.17)$$

where $C = 0.57721\dots$ is the Euler constant (we have used an unconventional symbol here to avoid the confusion with the friction constant γ), (2.15) may be written

$$\frac{\partial}{\partial \gamma} \langle x^2 \rangle = -\frac{\hbar^3}{4 \pi^3 m (kT)^2} \operatorname{Re} \left[\sum_{n=1}^{\infty} \frac{n}{(n+z_1)^2 (n+z_2)^2} \right]. \quad (2.18)$$

Similarly,

$$\frac{\partial}{\partial K} \langle x^2 \rangle = -\frac{\hbar^4}{8 \pi^4 m^2 (kT)^3} \operatorname{Re} \left[\frac{1}{2(z_1 z_2)^2} + \sum_{n=1}^{\infty} \frac{1}{(n+z_1)^2 (n+z_2)^2} \right]. \quad (2.19)$$

Since from (2.3) and (2.10), z_1 and z_2 are either complex conjugates of each other (if $\omega_0 > \gamma/2$) or two real positive quantities (if $\omega_0 < \gamma/2$), the summands within the brackets in (2.18) and (2.19) are all real positive quantities. Therefore we conclude that

$$\frac{\partial}{\partial \gamma} \langle x^2 \rangle < 0, \quad (2.20)$$

and that

$$\frac{\partial}{\partial K} \langle x^2 \rangle < 0. \quad (2.21)$$

We conclude that in the case of an *Ohmic* heat bath, *at arbitrary temperature*, the mean square displacement of a quantum oscillator monotonically decreases (so that *the oscillator becomes more localized*) with *increasing γ or K* .

It is also of interest to check the $\gamma \rightarrow 0^+$ limit of $\langle x^2 \rangle$. In the absence of a heat bath, (2.10) now becomes $z_{1,2} = \pm i\hbar\omega_0/2\pi kT$. By using the recursion formula for $\psi(z)$, $\psi(z+1) = \psi(z) + 1/z$, and its reflection formula, $\psi(1-z) = \psi(z) + \pi \cot(\pi z)$, (2.12) can be reduced to

$$\langle x^2 \rangle = \frac{\hbar}{2m\omega_0} \coth\left(\frac{\hbar\omega_0}{2kT}\right), \quad (2.22)$$

which is exactly the result for a free quantum oscillator at temperature T .

III. Blackbody Radiation Heat Bath

In this case, the spectral distribution function is [82 – 84]

$$\bar{\mu}(\omega) = 2e^2\Omega^2\omega/3c^3(\omega + i\Omega), \quad (3.1)$$

where Ω is a large cutoff frequency.

Here one must be careful to go to the large-cutoff limit only after the completion of the integral in (1.6). The order can be of importance in some cases, as will be shown later in the calculation. [In particular, note the $\ln m$ term in (3.13) which is divergent in the large-cutoff limit.]

Putting (3.1) into (1.3) and factoring the denominator, we have [83,84]

$$\alpha(\omega) = \frac{\omega + i\Omega}{m(\omega + i\Omega')(\omega_0^2 - \omega^2 - i\gamma\omega)}, \quad (3.2)$$

where the introduced parameters Ω' , ω_0 , and γ satisfy the relations

$$\frac{1}{\Omega} = \frac{1}{\Omega'} + \frac{\gamma}{\omega_0^2}, \quad \frac{K}{m} = \frac{\omega_0^2 \Omega'}{\Omega' + \gamma}, \quad \frac{M}{m} = \frac{(\gamma \Omega' + \omega_0^2)(\Omega' + \gamma)}{\omega_0^2 \Omega'}, \quad (3.3)$$

where

$$M = m + 2e^2 \Omega / 3c^3 \quad (3.4)$$

is the renormalized mass.

In partial-fraction form, (3.2) becomes

$$\alpha(\omega) = \frac{A}{\omega + i\Omega'} + \frac{B}{\omega + i\omega_1} + \frac{C}{\omega + i\omega_2}, \quad (3.5)$$

where

$$\omega_{1,2} = \frac{1}{2} \gamma \pm i \sqrt{\omega_0^2 - \frac{1}{4} \gamma^2}, \quad (3.6)$$

and

$$\begin{aligned} A &= \frac{i(\Omega - \Omega')}{m(\omega_0^2 + \Omega'^2 - \gamma\Omega')}, & B &= \frac{i(\Omega - \omega_1)}{m(\Omega' - \omega_1)(\omega_2 - \omega_1)}, \\ C &= \frac{i(\Omega - \omega_2)}{m(\Omega' - \omega_2)(\omega_1 - \omega_2)}. \end{aligned} \quad (3.7)$$

From (3.7), it can be readily shown that

$$A + B + C = 0. \quad (3.8)$$

The imaginary part of $\alpha(\omega)$, from (3.5), is

$$\text{Im } \alpha(\omega) = \omega \text{Im} \left(\frac{A}{\omega^2 + \Omega'^2} + \frac{B}{\omega^2 + \omega_1^2} + \frac{C}{\omega^2 + \omega_2^2} \right). \quad (3.9)$$

In the large-cutoff limit ($\Omega' \gg \gamma$ and $\Omega' \gg \omega_0$), the first terms in (3.5) and (3.9) are negligible and we remark that similar limits are obtained if one first took the large-cutoff limit in $\alpha(\omega)$ itself.

Substituting (3.9) into (1.6) and using (3.8), we obtain

$$\langle x^2 \rangle \Big|_{T=0} = \frac{\hbar}{\pi} \int_0^\infty d\omega \text{Im } \alpha(\omega) = -\frac{\hbar}{\pi} \text{Im} (A \ln \Omega' + B \ln \omega_1 + C \ln \omega_2). \quad (3.10)$$

Now we may pass to the large-cutoff limit ($m \rightarrow 0$), which from (3.3), (3.4), and (3.7) can be shown to give

$$\Omega' = \frac{M}{m\tau_e} [1 + O(m/M)], \quad \omega_0^2 = \frac{K}{M} + O(m/M), \quad \gamma = \omega_0^2 \tau_e + O(m/M), \quad (3.11)$$

where $\tau_e \equiv 2e^2/3Mc^3$; and

$$\begin{aligned} A &= -\frac{i\tau_e}{M} + O(m/M), & B &= \frac{i\omega_1^2}{M\omega_0^2(\omega_1 - \omega_2)} + O(m/M), \\ C &= \frac{i\omega_2^2}{M\omega_0^2(\omega_2 - \omega_1)} + O(m/M). \end{aligned} \quad (3.12)$$

The omitted terms are all of the order of m/M . From the last of Eqs. (3.11), it is clear that γ is a function of ω_0 , and hence *the only independent parameters in this problem are T and ω_0* . In fact for $m \rightarrow 0$, it is clear from (3.10) to (3.12) that the integral expression for $\langle x^2 \rangle$ in the blackbody radiation case is the same as that in the Ohmic case except for an extra factor of ω^2/ω_0^2 in the integrand, which results in a linear divergent integral in the blackbody case. However, if the integration is performed before the large

cutoff limit is taken (which is the preferred procedure), then a logarithmically divergent result is obtained [see (3.13)].

Let us, first of all, examine the zero-temperature case. Using (3.11) and (3.12) in (3.10), we obtain

$$\begin{aligned} \langle x^2 \rangle|_{T=0} &= \frac{\hbar \tau_e}{\pi M} \ln\left(\frac{M}{m}\right) - \frac{\hbar \tau_e}{\pi M} \ln \tau_e + \frac{\hbar}{2\pi M \omega_0^2} \operatorname{Im} \left[\frac{1}{\sqrt{\omega_0^2 - \gamma^2/4}} (\omega_2^2 \ln \omega_2 - \omega_1^2 \ln \omega_1) \right] \\ &= \frac{\hbar \tau_e}{\pi M} \ln\left(\frac{M}{m}\right) - \frac{\hbar \tau_e}{\pi M} \ln(\omega_0 \tau_e) + \frac{\hbar}{\pi M \omega_0^2} \left[\frac{\omega_0^2 - \gamma^2/2}{\sqrt{\omega_0^2 - \gamma^2/4}} \tan^{-1} \left(\frac{2}{\gamma} \sqrt{\omega_0^2 - \gamma^2/4} \right) \right]. \end{aligned} \quad (3.13)$$

The first term in the above equation, though logarithmically divergent as $m \rightarrow 0$, is independent of K (or ω_0^2), and therefore $(\partial/\partial K) \langle x^2 \rangle|_{T=0}$ is finite:

$$\frac{\partial}{\partial K} \langle x^2 \rangle|_{T=0} = -\frac{\hbar}{2\pi K^2} \left[\frac{\omega_0^2}{\sqrt{\omega_0^2 - \gamma^2/4}} \tan^{-1} \left(\frac{2}{\gamma} \sqrt{\omega_0^2 - \gamma^2/4} \right) + \frac{\gamma(3\omega_0^2 - \gamma^2)}{2(\omega_0^2 - \gamma^2/4)} \right], \quad (3.14)$$

which is negative by the inequalities

$$\tan^{-1} x > x(1 - 3x^2) / (1 + x^2)^2 \quad (x > 0) \quad (3.15)$$

and

$$\frac{1}{2} \ln[(1+x)/(1-x)] < x(1 + 3x^2) / (1 - x^2)^2 \quad (0 < x < 1). \quad (3.16)$$

In other words, in the case of a blackbody radiation heat bath at zero temperature, localization is enhanced due to increased K .

Equations (3.13) and (3.14) are valid for $\omega_0 > (\gamma/2)$. In the case of $\omega_0 < (\gamma/2)$, one needs just to replace $(\omega_0^2 - \gamma^2/4)^{-1/2} \tan^{-1} \left[(2/\gamma)(\omega_0^2 - \gamma^2/4)^{1/2} \right]$ by

$$\frac{1}{2\sqrt{\gamma^2/4 - \omega_0^2}} \ln \left(\frac{\gamma/2 + \sqrt{\gamma^2/4 - \omega_0^2}}{\gamma/2 - \sqrt{\gamma^2/4 - \omega_0^2}} \right),$$

according to the identity

$$\tan^{-1}(ix) = \frac{1}{2}i \ln[(1+x)/(1-x)] . \quad (3.17)$$

We now turn to the case of nonzero temperature. For the temperature-dependent part of $\langle x^2 \rangle$, the contribution due to the first term of $\text{Im } \alpha(\omega)$ in (3.9), when inserted in (2.7), is

$$\frac{\hbar}{\pi} \text{Im} \left\{ A \left[\ln \left(\frac{\hbar \Omega'}{2\pi kT} \right) - \psi \left(\frac{\hbar \Omega'}{2\pi kT} \right) - \frac{\pi kT}{\hbar \Omega'} \right] \right\} , \quad (3.18)$$

which, by using the asymptotic expansion of $\psi(z)$,

$$\psi(z) \sim \ln z - \frac{1}{2z} - \frac{1}{12z^2} \dots \quad (z \rightarrow \infty \text{ in } |\arg z| < \pi) , \quad (3.19)$$

approaches to $(\hbar/\pi) \text{Im} [(A/12)(2\pi kT/\hbar \Omega')^2] \rightarrow 0$ as $\Omega' \rightarrow \infty$ (or, equivalently, $m \rightarrow 0$). Thus, to calculate $\Delta \langle x^2 \rangle$, one might simply take the large-cutoff limit in $\alpha(\omega)$ first before the integration. This is valid here because the resulting integral is finite, hence the order of limiting and integrating can be exchanged.

Combining the remaining two terms in (3.9) with (2.8) and (2.11), we obtain

$$\Delta \langle x^2 \rangle = \frac{2\pi(kT)^2}{\hbar M \omega_0^2} \text{Im} \left\{ \frac{1}{\sqrt{\omega_0^2 - \gamma^2/4}} \left[z_1^2 (\ln z_1 - \psi(z_1)) - \frac{1}{2} z_1 - z_2^2 (\ln z_2 - \psi(z_2)) + \frac{1}{2} z_2 \right] \right\} , \quad (3.20)$$

where z_1 and z_2 are again given by (2.10), with γ understood to be satisfying (3.11).

In the high-temperature limit, this expression becomes

$$\Delta \langle x^2 \rangle = \frac{kT}{M \omega_0^2} - \frac{\hbar \tau_e}{\pi M} \ln \left(\frac{2\pi kT}{\hbar \omega_0} \right) + \dots , \quad (3.21)$$

while in the low-temperature limit, it becomes

$$\Delta\langle x^2 \rangle = \frac{2\pi^3 \tau_e (kT)^4}{15 \hbar^3 M \omega_0^4} + \dots \quad (3.22)$$

Next consider the $\omega_0 \tau_e \ll 1$ limit, which is true in most circumstances, since τ_e is typically exceedingly small ($\tau_e = 6.27 \times 10^{-24}$ sec. in the case of the electron). Then

$$\langle x^2 \rangle|_{T=0} = \frac{\hbar \tau_e}{\pi M} \ln\left(\frac{M}{m \omega_0 \tau_e}\right) + \frac{\hbar}{\pi M \omega_0} \left[\frac{1}{2} \pi - \frac{1}{2} \omega_0 \tau_e - \frac{3}{16} \pi (\omega_0 \tau_e)^2 + \dots \right] \quad (3.23)$$

and

$$\begin{aligned} \Delta\langle x^2 \rangle = & \frac{\hbar}{M \omega_0 [\exp(\hbar \omega_0 / kT) - 1]} + \omega_0 \tau_e \left\{ \frac{\hbar}{\pi M \omega_0} \ln\left(\frac{\hbar \omega_0}{2\pi kT}\right) \right. \\ & \left. + \frac{\hbar}{2\pi M \omega_0} - \frac{\hbar}{\pi M \omega_0} \operatorname{Re} \left[\psi(z_0) + \frac{1}{2} z_0 \psi'(z_0) \right] \right\} + O(\omega_0 \tau_e)^2, \end{aligned} \quad (3.24)$$

where $z_0 \equiv i\hbar \omega_0 / 2\pi kT$.

Finally, taking the derivative of $\langle x^2 \rangle$ with respect to K , we have

$$\begin{aligned} \frac{\partial}{\partial K} \langle x^2 \rangle = & \frac{\partial}{\partial K} \langle x^2 \rangle|_{T=0} + \frac{\partial}{\partial K} \Delta\langle x^2 \rangle \\ = & \frac{\hbar}{4\pi K^2 (\omega_0^2 - \gamma^2/4)} \operatorname{Im} \left\{ i \left[z_2 \omega_2^3 \psi'(z_2) + z_1 \omega_1^3 \psi'(z_1) \right] \right. \\ & \left. + \frac{\omega_0^4}{\sqrt{\omega_0^2 - \gamma^2/4}} [\psi(z_2) - \psi(z_1)] \right\} + \frac{kT}{K^2}. \end{aligned} \quad (3.25)$$

By the same technique used in section II, one may show that

$$\frac{\partial}{\partial K} \langle x^2 \rangle = -\frac{2kT}{K^2} \left\{ \frac{1}{2} + \sum_{n=1}^{\infty} \left[\frac{(z_1 + z_2)n + z_1 z_2}{(n + z_1)(n + z_2)} \right]^2 \right\} < 0. \quad (3.26)$$

We conclude that, in the case of a *blackbody radiation heat bath*, at any temperature, *the localization is enhanced due to increasing K* (i.e., increased binding). A similar result holds in the case of increasing dissipation since γ is proportional to K .

IV. Conclusions

In the case of an arbitrary spectral distribution we have shown that localization increases with decreasing temperature. Also, we have shown that, in the case of an Ohmic heat bath and a blackbody radiation heat bath, at any temperature, either increase of dissipation or increase of binding leads to an enhancement of localization.

CHAPTER III

ON THE QUANTUM DISSIPATIVE SYSTEM OF A CHARGED PARTICLE MOVING IN A MAGNETIC FIELD AND IN A HEAT BATH

1. Introduction to Chapter III

Chapter III of this dissertation is devoted to the study of the three-dimensional (3D) motion of a charged quantum particle coupled linearly to a heat bath, in the presence of an external magnetic field as well as a binding potential [116,131].

The problem of isolated charged particles diffusing under an applied magnetic field and coupled to a neutral background medium, in two dimensions (2D), occurs in many contexts in condensed-matter physics. The early research topics cover the influence of collisions on the magnetic susceptibility of metals [132,133]; quantum transport theory of an electron gas in a magnetic field [134]; magnetoresistance on the Fermi surface [135,136]; electronic conduction in a strong magnetic field [137,138]; nuclear magnetic resonance (NMR) [139]; relaxation and resonance of spins in zero or low external magnetic fields [140,141]; electron-hole pair production and recombination in semiconductors [142]; diffusion of nondegenerate charge carriers in a semiconductor [143]; and magnetopolaron (i.e., the Fröhlich polaron in the presence of an external magnetic field) [144]. The techniques employed in these studies are predominantly the phase-space Fokker-Planck equation for the Wigner function, with the influence of the ambient medium being taken into account only phenomenologically [145].

Interest in the subject has been revived over the last decade or so. More recent examples include the unusual temperature dependence of the Hall angle for lattice polarons and holes in spin-disordered backgrounds [146]; charged interstitials in normally conducting metals [147]; highly nonclassical transport of a degenerate Fermi gas in the

presence of strong disorder in the quantized Hall effect [148]; temperature-dependent normal-state Hall effect in the quasi-two-dimensional system of high-temperature cuprate superconductors (and some heavy-fermion compounds) caused by strong inelastic scattering [149]; macroscopic magnetization tunneling [150]; and Hall mobility and diamagnetism of a 2D charged gas in the dissipative regime [151].

In Ref. 152, the body text of which constitutes Section 2 of this dissertation, the 1D problem of a quantum particle moving in an arbitrary scalar potential and coupled linearly to a passive heat bath is generalized to the 3D version of a charged particle in the presence of an additional external magnetic field, with the heat bath composed of independent, neutral harmonic oscillators. The static magnetic field is accommodated in the formulation through the well-known minimal coupling rule and is shown, by a general gauge-independent derivation within the IO model, to manifest itself by the presence of an extra term in the GLE which is the quantum version of the Lorentz force, but leaves both the memory function and the random force appearing in the GLE unaffected. Consequently, the noise-noise autocorrelation function, as well as the nonequal time commutator of the noise, remains the same. That the dissipation and the external force do not affect each other is characteristic of the linear coupling between the particle and the heat bath assumed in the model [153,154]. The corresponding Schrödinger–Langevin equation implies that the Aharonov–Bohm effect is also not influenced by the dissipation [153]. Since the formulation presented incorporates amply the effects of Landau-orbit quantization and the corresponding Landau-level structure, no semiclassical approximation is necessary. The linearity of the coupling between particle and heat bath adopted in the IO model allows the magnetic field to be taken into account nonperturbatively.

The general formalism thus developed is applied to tackle the problem of a harmonically bound, charged quantum Brownian particle in the presence of a constant, homogeneous magnetic field [155]. (The body text of Ref. 155 constitutes Section 3 of this

dissertation.) There, the generalized susceptibility tensor, which plays an essential role in determining the dynamics of the system, is solved for exactly from the ensuing linear differential equation of motion by means of the Fourier transformation. It is then used to obtain the symmetrized position correlation functions by means of the fluctuation–dissipation (FD) theorem. The free energy of the oscillator, defined as the free energy of the system-plus-reservoir complex minus that of the heat bath itself, is derived in terms of the determinant of the generalized susceptibility matrix and evaluated explicitly for the Ohmic as well as the blackbody radiation heat baths. This remarkable formula for the free energy may be elucidated by a more intuitive analysis that interprets the zeros and poles of the determinant of the generalized susceptibility matrix as the normal-mode frequencies of the heat bath itself and of the system-plus-reservoir complex, respectively. As an interesting by-product, the well-known eigenspectrum of a charged oscillator in a magnetic field is recovered as a special case by removing the heat bath from the formula. The significance of the free energy formula may further be appreciated by noting that the derivatives of free energy with respect to circular frequency of the oscillator and magnetic field yield, through the Hellman–Feynman theorem [156], the mean square displacement and the magnetic moment of the charged oscillator, respectively. The latter relation could be used to probe the magnetism of a single charged oscillator or Brownian particle in a heat bath (see Ref. 158, Appendix D).

The effect of dissipation on a charged quantum harmonic oscillator in the presence of an external magnetic field is considered in Ref. 157 (the body text of which constitutes Section 4 of this dissertation), and found to give rise to unexpected results, owing to the complicated interplay between the magnetic field and the dissipation. Unlike the corresponding 1D situation where dissipation always enhances localization [125], one discovers here that, at least at zero temperature, the magnetic field instead tends to delocalize the oscillation in the plane perpendicular to it when it is stronger than a critical

value. This somewhat puzzling result may be related to the discovery in the research work on magnetopolarons [144] that an ideal gas of polarons can undergo a magnetic phase transition. At the transition point and with increasing magnetic field strength, the polaron gas transforms from a polaron state to an almost free Landau state in the direction normal to the magnetic field. Hence, this conversion may be viewed as a 2D stripping of the polaron induced by the magnetic field.

In Ref. 158 (the body text of which constitutes Section 5 of this dissertation), we expand the work presented in Ref. 155 and, in particular, focus our attention on two important quantities frequently employed in the study of condensed matter: the retarded Green's functions and the symmetrized position correlation functions. They play prominent roles in the theoretical interpretation of experiments because of their direct relationship with measurable physical quantities and thus are the subject of much interest [44,117].

In that paper, we start by first introducing the general formalism and notation used. In particular, we establish several useful properties of the generalized susceptibility tensor obtained from the GLE for an isotropic harmonic oscillator. We then define the retarded Green's functions as the Fourier transform of the generalized susceptibility tensor and relate them to the nonequal time commutators of position operators. Owing to the linear nature of the coupling between particle and heat bath in the IO model, the retarded Green's functions so constructed are temperature independent and are connected with the symmetrized position correlation functions through the fluctuation-dissipation theorem (FD). For linear systems as are discussed here, all higher-order correlation functions can simply be factorized into summations of pair correlation functions due to the Gaussian properties of the underlying stochastic processes [63,78,82,104]. This relation between the retarded Green's functions and the symmetrized position correlation functions allows us to prove, based on the properties of generalized susceptibility tensors

mentioned above, two general theorems, concerning the position autocorrelation functions (dispersions) of motions vertical to the external magnetic field, that are true for any physical heat baths. Besides the transversal dispersions of a charged quantum particle, the free energy of such a system has also been shown to decrease monotonically with increasing magnetic field strength, hence indicating the diamagnetism of the system despite the presence of an arbitrary heat bath. The generality of these theorems originates from the fact that, because of the neutrality of the independent oscillators of the heat bath implied in the IO model, the magnetic field enters into the GLE only through the Lorentz-force term so that the external field and the dissipation do not affect each other. It may be of interest to note in this regard a similar theorem on the magnetoconductivity of metals that states under rather general assumptions that if an external magnetic field has no bearing on scattering mechanisms, then the electric conductivity of metals is a monotonically nonincreasing function of the magnitude of the magnetic field [159]. We have also calculated explicitly the retarded Green's functions and the symmetrized position correlation functions for a harmonic oscillator in the Ohmic heat bath, in both classical and quantum domains.

We have also extended the investigation, in Ref. 158, to the Brownian motion of a charged particle in an external magnetic field. To deduce finite results, we introduce the displacement correlation functions, which are related to the symmetrized position correlation functions but are more appropriate for studying the Brownian motion. We then present a formula for the self-diffusion constant and derive, in the limit of long times at both absolute zero (the quantum regime) and nonzero temperatures (the classical regime), two general relations between the retarded Green's functions and the displacement correlation functions. The classical version of the two is a generalization of the Einstein relation and can thus be cast into the form of the Green-Kubo formulas connecting transport coefficients with integrals of appropriate correlation functions. The formulas developed

in this way are subsequently applied to extract the long-time asymptotic expansion of the displacement correlation functions from that of the retarded Green's functions, for the Ohmic heat bath and a rather general class of frequency-dependent heat baths corresponding to many realistic microscopic models and therefore having been studied extensively, particularly in the context of dissipative quantum phase coherence [99]. As in the non-magnetic case, well-separated time scales, which are required for the interpretation in terms of a standard Brownian motion, appear only in the high-temperature (classical) regime. In the opposite limit of low temperature, the interplay between quantum and thermal fluctuations prevails, leading to long-time tails of the inverse-square-law form in the time correlation functions [160]. We have shown that the functional dependencies on time of both the retarded Green's functions and the displacement correlation functions are unchanged by the magnetic field; only the overall coefficients are reduced by it for transverse motions. Hence a static magnetic field can not confine a charged particle coupled to an Ohmic heat bath, not even at absolute zero temperature. It only slows down transverse diffusion [131]. For the sub-Ohmic case where damping dominates at low frequencies (or, equivalently, at long times), an initially localized state remains localized at zero temperature, even without an external potential, because of a finite variance. Thereby the transverse localization length is shorter than the longitudinal one.

The method and results presented may also be useful in studying magnetic properties such as the diamagnetic susceptibility, magnetoconductivity, and Hall coefficient for a two-dimensional (2D) system of charged particles in the dissipative (or incoherent) regime. One example of a quasi-2D system associated with the quantized Hall effect is the degenerate electron fluids generated as inversion layers at semiconductor surfaces in the presence of strong disorder. Another one is the normal state of low-temperature cuprate superconductors. Since either Bose or Fermi statistics yields only perturbative corrections in the dissipative regime [161] and since two-body interactions do not alter the

amplitude and period of the de Haas–van Alphen oscillations as well as the total magnetic moment of a system of interacting fermions [162], the GLE approach for the problem of a single charged Brownian particle could be applicable to such systems.

The reprints of Refs. 152 and 155 and the preprints of Refs. 157 and 158 cited above form Sections 2, 3, 4, and 5, respectively, in Chapter III of this dissertation.

2. Magnetic-Field Effects on the Motion of a Charged Particle in a Heat Bath*

I. Introduction

The problem of a quantum particle coupled to a quantum-mechanical heat bath can be formulated in terms of the quantum Langevin equation. The quantum Langevin equation is a macroscopic equation corresponding to a reduced description of the system in which the coupling with the heat bath is described by two terms: an operator-valued random force $F(t)$ with mean zero, and a mean force characterized by a memory function $\mu(t)$.

Ford, Lewis, and O'Connell (FLO) [82] have shown that the most general quantum Langevin equation can be realized by the independent-oscillator (IO) model of a heat bath. It is a simple and convenient model with which to calculate. Yet by suitably choosing the distribution of the frequencies and force constants for the independent oscillators, one can represent the most general positive real function, and through it the general macroscopic description of the heat-bath problem.

In this paper, we extend the work of FLO to include the presence of a static external magnetic field. What we find is that the only influence of the magnetic field on a charged particle occurs through the addition of an extra term in the quantum Langevin equation (which is the quantum version of the classical Lorentz force), and that the memory function and the random force are unchanged by the magnetic field. A similar problem has previously been considered by Marathe [131], but that work did not include an

*This section consists of the body text of Ref. 152, by X. L. Li, G. W. Ford, and R. F. O'Connell, with its abstract incorporated in Sec. 1 (Introduction to Chapter III) and its references merged into the overall bibliography. This research was partially supported by the U. S. Office of Naval Research, Grant No. N00014-90-J-1124.

external potential; the derivation of the equation of motion implied a special gauge for the vector potential \vec{A} and a special choice of the memory function was made in calculating such quantities as the noise-noise autocorrelation function.

In Sec. II we give a general, gauge-independent calculation of the contribution of the external magnetic field to the quantum Langevin equation in the IO model. As has been stressed by FLO, although we utilize the IO model, the equations obtained transcend this model. Next, we calculate the noise-noise autocorrelation function, as well as the nonequal time commutator of the noise, for an arbitrary memory function. In Sec. III we present our conclusions and we discuss briefly the blackbody radiation field heat-bath model (BBR) as an example of the generality of the results we have obtained.

II. The Independent-Oscillator Model in a Magnetic Field

Our working model is the IO model, in which a charged particle moves in an external magnetic field and in an arbitrary potential, and is linearly coupled to a large (eventually infinite) number of heat-bath particles [82]. The Hamiltonian of the system is then

$$H = \frac{1}{2m} \left[\vec{p} - \frac{e}{c} \vec{A} \right]^2 + V(\vec{r}) + \sum_j \left[\frac{\vec{p}_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 (\vec{q}_j - \vec{r})^2 \right], \quad (1)$$

where e , m , \vec{r} , and \vec{p} are the charge, mass, position, and momentum of the particle, respectively, and $V(\vec{r})$ denotes the external potential. The j th heat-bath particle has a mass m_j , frequency ω_j , position \vec{q}_j , and momentum \vec{p}_j . The vector potential $\vec{A}(\vec{r})$ is related to the magnetic field $\vec{B}(\vec{r})$ by the equation

$$\vec{B}(\vec{r}) = \vec{\nabla}_{\vec{r}} \times \vec{A}(\vec{r}). \quad (2)$$

The commutation rules for the various position and momentum operators are, as usual,

$$\left[r_\alpha, p_\beta \right] = i\hbar \delta_{\alpha\beta}, \quad \left[q_{j\alpha}, p_{k\beta} \right] = i\hbar \delta_{jk} \delta_{\alpha\beta}, \quad (3)$$

and all other commutators vanish.

Without the \bar{A} field, (1) is just the Hamiltonian considered in the FLO paper [82]. In the presence of an external magnetic field, the motion of the charged particle is generally three dimensional. This necessitates the vector notations in the Hamiltonian. In the following vector analysis, the Greek indices stand for three spatial directions (i.e., $\alpha, \beta, \dots = 1, 2, 3$) and the Roman indices i, j, k denote the different heat-bath particles.

The Heisenberg equations of motion for the heat-bath particles from (1) are

$$\begin{aligned} \dot{\bar{q}}_j &= [\bar{q}_j, H]/i\hbar = \bar{p}_j/m_j, \\ \dot{\bar{p}}_j &= [\bar{p}_j, H]/i\hbar = -m_j \omega_j^2 (\bar{q}_j - \bar{r}). \end{aligned} \quad (4)$$

These combine to give

$$\ddot{\bar{q}}_j + \omega_j^2 \bar{q}_j = \omega_j^2 \bar{r}, \quad (5)$$

where the dot denotes the derivative with respect to t .

For the charged particle, the equations of motion are

$$\dot{\bar{v}} \equiv \dot{\bar{r}} = [\bar{r}, H]/i\hbar = \left[\bar{p} - \frac{e}{c} \bar{A} \right] / m, \quad (6)$$

$$\begin{aligned} \dot{p}_\alpha &= [p_\alpha, H]/i\hbar \\ &= \frac{1}{2mi\hbar} \left[p_\alpha, \left(\bar{p} - \frac{e}{c} \bar{A} \right)^2 \right] - \partial_\alpha V + \sum_j m_j \omega_j^2 (q_{j\alpha} - r_\alpha), \end{aligned} \quad (7)$$

where $\partial_\alpha \equiv \partial/\partial r_\alpha$ is the spatial derivative.

The first term on the right-hand side of (7) may be written as

$$\frac{1}{2mi\hbar} \left[p_\alpha, \left(\bar{p} - \frac{e}{c} \bar{A} \right)^2 \right] = \frac{e}{2c} \left[v_\beta \partial_\alpha A_\beta + (\partial_\alpha A_\beta) v_\beta \right], \quad (8)$$

where the Einstein summation convention applies to repeated indices. Now

$$\begin{aligned} (\partial_\alpha A_\beta) v_\beta &= v_\beta \partial_\alpha A_\beta + \frac{1}{m} [\partial_\alpha A_\beta, p_\beta] \\ &= v_\beta \partial_\alpha A_\beta + \frac{i\hbar}{m} \partial_\alpha \partial_\beta A_\beta, \end{aligned} \quad (9)$$

and

$$(\bar{v} \times \bar{B})_\alpha = v_\beta \partial_\alpha A_\beta - v_\beta \partial_\beta A_\alpha. \quad (10)$$

Combining (8), (9), and (10), we have

$$\frac{1}{2mi\hbar} \left[p_\alpha, \left(\bar{p} - \frac{e}{c} \bar{A} \right)^2 \right] = \frac{e}{c} (\bar{v} \times \bar{B})_\alpha + \frac{e}{c} v_\beta \partial_\beta A_\alpha + \frac{i\hbar e}{2mc} \partial_\alpha \partial_\beta A_\beta. \quad (11)$$

In vector form, (7) thus becomes

$$\dot{\bar{p}} = -\bar{\nabla} V(\bar{r}) + \sum_j m_j \omega_j^2 (\bar{q}_j - \bar{r}) + \frac{e}{c} (\bar{v} \times \bar{B}) + \frac{e}{c} (\bar{v} \cdot \bar{\nabla}) \bar{A} + \frac{i\hbar e}{2mc} \bar{\nabla} (\bar{\nabla} \cdot \bar{A}). \quad (12)$$

Similarly,

$$\dot{\bar{A}}(\bar{r}) = \frac{\partial}{\partial t} \bar{A} + \frac{1}{i\hbar} [\bar{A}, H] = (\bar{v} \cdot \bar{\nabla}) \bar{A} + \frac{i\hbar}{2m} \nabla^2 \bar{A}, \quad (13)$$

where we have used the static condition $\partial \bar{A} / \partial t = 0$.

Eliminating the momentum variables in (6) and (12), and using (13), we get

$$m\ddot{\bar{r}} = -\bar{\nabla} V(\bar{r}) + \sum_j m_j \omega_j^2 (\bar{q}_j - \bar{r}) + \frac{e}{c} (\bar{v} \times \bar{B}) + \frac{i\hbar e}{2mc} [\bar{\nabla} (\bar{\nabla} \cdot \bar{A}) - \nabla^2 \bar{A}]. \quad (14)$$

But, from electromagnetism, we know that

$$\bar{\nabla} (\bar{\nabla} \cdot \bar{A}) - \nabla^2 \bar{A} = \frac{4\pi}{c} \bar{j},$$

where \vec{j} is the source current of the external magnetic field. In practice, it lies outside the region where the charged particle moves. Thus the last term in (14) vanishes and (14) becomes

$$m\ddot{\vec{r}} = -\vec{\nabla}V(\vec{r}) + \sum_j m_j \omega_j^2 (\vec{q}_j - \vec{r}) + \frac{e}{c} (\vec{v} \times \vec{B}). \quad (15)$$

Here we see that the only effect of the magnetic field is the $(e/c)(\vec{v} \times \vec{B})$ term, which is the quantum generalization of the classical Lorentz force. We note that (15) is gauge independent.

The retarded solution of (5) is

$$\vec{q}_j(t) = \vec{q}_j^h(t) + \vec{r}(t) - \int_{-\infty}^t dt' \cos[\omega_j(t-t')] \dot{\vec{r}}(t'), \quad (16)$$

where $\vec{q}_j^h(t)$ is the general solution of the homogeneous equation of (5) ($\vec{r} \equiv 0$).

Substituting (16) in (15) we get the generalized quantum Langevin equation

$$m\ddot{\vec{r}} + \int_{-\infty}^t dt' \mu(t-t') \dot{\vec{r}}(t') + \vec{\nabla}V(\vec{r}) - \frac{e}{c} (\dot{\vec{r}} \times \vec{B}) = \vec{F}(t), \quad (17)$$

with the memory function and the random force the same as those given in the FLO paper:

$$\mu(t) = \sum_j m_j \omega_j^2 \cos(\omega_j t) \theta(t), \quad (18)$$

$$\vec{F}(t) = \sum_j m_j \omega_j^2 \vec{q}_j^h(t). \quad (19)$$

Thus (17) is the same as the FLO result except for the last term on the left-hand side of (17). One immediate conclusion is that the symmetric autocorrelation as well as the nonequal time commutator of $\vec{F}(t)$ are the same as those in the absence of the \vec{B} field [82]:

$$\begin{aligned} & \frac{1}{2} \langle F_\alpha(t) F_\beta(t') + F_\beta(t') F_\alpha(t) \rangle \\ &= \delta_{\alpha\beta} \frac{1}{\pi} \int_0^\infty d\omega \operatorname{Re} [\tilde{\mu}(\omega + i0^+)] \hbar \omega \coth\left(\frac{\hbar\omega}{2kT}\right) \cos[\omega(t-t')] , \end{aligned} \quad (20)$$

$$[F_\alpha(t), F_\beta(t')] = \delta_{\alpha\beta} \frac{2}{i\pi} \int_0^\infty d\omega \operatorname{Re} [\tilde{\mu}(\omega + i0^+)] \hbar \omega \sin[\omega(t-t')] , \quad (21)$$

where

$$\tilde{\mu}(z) \equiv \int_0^\infty dt e^{iz} \mu(t) \quad (22)$$

and

$$\operatorname{Re} [\tilde{\mu}(\omega + i0^+)] = \frac{\pi}{2} \sum_j m_j \omega_j^2 [\delta(\omega - \omega_j) + \delta(\omega + \omega_j)] . \quad (23)$$

III. Conclusions

We have seen that the equation of motion of a charged particle in a heat bath, moving in an arbitrary potential and in an external magnetic field, can still be written in the form of a generalized quantum Langevin equation, with the influence of the magnetic field being exhibited solely by a single extra term, which is the quantum version of the Lorentz force.

In contrast to the corresponding results of Marathe [131], our results are very general in the sense that (a) they are gauge invariant (a special choice of gauge is implied for the vector potential \bar{A} in Ref. 131); (b) they include the case of an arbitrary external potential $V(\bar{r})$; and (c) they apply to any choice of memory function [whereas in Ref. 131 a specific choice of $\mu(t)$ was made, as can be seen from Eq. (2.9) of that paper, and noting that the memory function there is denoted by $K(t)$].

The generality of our results has one immediate consequence, viz., they can be applied to get the corresponding results in a case of much physical interest, viz., the blackbody radiation (BBR) heat bath [82,83]. By means of a series of unitary transformations, FLO have shown the equivalence of the BBR and IO heat-bath models in the

absence of a magnetic field [82]. It turns out that exactly the same transformations apply in the present case. The key point is that the unitary transformations leave \vec{r} unchanged, so that the $-(e/c)(\dot{\vec{r}} \times \vec{B})$ term in the equation of motion also remains unchanged. In other words, in the case of the BBR heat bath, we can use (17) as it stands, with the explicit forms for $\mu(t)$ and $\vec{F}(t)$ being unchanged from the $B=0$ results [see FLO, Eqs. (5.16) and (5.12) for the explicit respective expressions].

3. Charged Oscillator in a Heat Bath in the Presence of a Magnetic Field*

I. Introduction

The problem of a charged quantum particle moving in an external magnetic field \vec{B} and in an arbitrary potential $V(\vec{r})$, and linearly coupled to a passive heat bath (consisting of an infinite number of oscillators) has been formulated in terms of the generalized quantum Langevin equation in an earlier paper [152]. The equation takes the form

$$m\ddot{\vec{r}} + \int_{-\infty}^t dt' \mu(t-t') \dot{\vec{r}}(t') + \bar{\nabla} V(\vec{r}) - \frac{e}{c} (\dot{\vec{r}} \times \vec{B}) = \vec{F}(t) , \quad (1.1)$$

where the dot denotes differentiation with respect to t . The influence of the external magnetic field is solely represented by the quantum version of the Lorentz-force term and both the operator-valued random force $\vec{F}(t)$ and the memory function $\mu(t)$ of the heat bath are unchanged by the magnetic field. In Ref. 152 we did not discuss susceptibilities, position autocorrelation functions, and free energies because their evaluation requires the specification of the potential. Here we discuss such quantities for the important case of a harmonic potential for which an exact analysis is possible.

In Sec. II we consider the problem of the response of the system to an external force $\vec{f}(t)$. In the case of a spatial harmonic potential, the problem is shown to be exactly

*This section consists of the body text of Ref. 155, by X. L. Li, G. W. Ford, and R. F. O'Connell, with its abstract incorporated in Sec. 1 (Introduction to Chapter III) and its references merged into the overall bibliography. This research was partially supported by the U. S. Office of Naval Research, Grant No. N00014-90-J-1124, and by the National Science Foundation, Grant No. INT-8902519.

solvable. The coefficient matrix of the response of the system to the perturbation, which is called the generalized susceptibility, plays an important role in determining the dynamics of the system. It is related to the correlation function of the position operator of the charged oscillator by the fluctuation–dissipation theorem. Furthermore, in the absence of the external force, it can be used to calculate the free energy of the oscillator in thermal equilibrium at temperature T , which is defined as the free energy of the system minus the free energy of the heat bath in the absence of the oscillator. The corresponding problem in the absence of a magnetic field has been considered by Ford, Lewis, and O’Connell [83]. They obtained this formula:

$$F_O(T) = \frac{1}{\pi} \int_0^\infty d\omega f(\omega, T) \text{Im} \left[\frac{d}{d\omega} \ln \alpha^{(0)}(\omega) \right], \quad (1.2)$$

where $f(\omega, T)$ is the free energy of a single oscillator of frequency ω at temperature T and $\alpha^{(0)}(\omega)$ is the scalar susceptibility in the absence of a magnetic field [83]. [It should be noted that, in Refs. 83 and 88, what we now call $\alpha^{(0)}(\omega)$ was referred to as $\alpha(\omega)$. The latter quantity now refers to the matrix of the elements $\alpha_{\rho\sigma}(\omega)$ as discussed below.]

In the presence of the external magnetic field, we shall show that the same formula holds only with $\alpha^{(0)}(\omega)$ replaced by the determinant of the generalized susceptibility matrix obtained in Sec. II. We will prove this in Sec. III by using the fluctuation–dissipation theorem. In the Appendix we present an alternative proof which is more succinct but perhaps less transparent. As we shall see, similar considerations apply to the case of the energy of the oscillator in thermal equilibrium at temperature T . In Sec. IV, we apply the general formulas obtained in Sec. III to two specific problems: the Ohmic and blackbody radiation heat baths. We shall see explicitly the diamagnetic behavior of the Ohmic heat bath at zero temperature. The blackbody radiation heat-bath problem is shown to be reducible to that of Ohmic heat bath plus a temperature-dependent shift in free energy. In Sec. V, we consider a special case (no heat bath) of our general formalism and obtain a

well-known eigenspectrum result, but in a simple and rather novel fashion. Finally, in Sec. VI, we present our conclusions.

II. Generalized Susceptibility for a Harmonic Potential

In the presence of an external force [88], the Hamiltonian has an added term $W = -\vec{r} \cdot \vec{f}(t)$, where $\vec{f}(t)$, the generalized force, is a given c-number function of time. This results in an added term $\vec{f}(t)$ on the right-hand side of (1.1). Thus, in a uniform external magnetic field and in a spatial harmonic potential well [$V(\vec{r}) = (1/2)K\vec{r}^2$], and in the presence of an external force $\vec{f}(t)$, the generalized quantum Langevin equation takes the form

$$m\ddot{\vec{r}} + \int_{-\infty}^t dt' \mu(t-t') \dot{\vec{r}}(t') - \frac{e}{c} (\dot{\vec{r}} \times \vec{B}) + K\vec{r} = \vec{F}(t) + \vec{f}(t) , \quad (2.1)$$

which is now a linear differential equation in \vec{r} . Fourier transforming (2.1), we obtain

$$\left[(-m\omega^2 - i\omega\tilde{\mu}(\omega) + K)\delta_{\rho\sigma} + i\omega\frac{e}{c}\epsilon_{\rho\sigma\eta}B_{\eta} \right] \tilde{r}_{\sigma}(\omega) = \tilde{F}_{\rho}(\omega) + \tilde{f}_{\rho}(\omega) , \quad (2.2)$$

where

$$\tilde{\mu}(\omega) \equiv \int_0^{\infty} dt e^{i\omega t} \mu(t) , \quad (2.3)$$

$$\tilde{r}_{\sigma}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} r_{\sigma}(t) , \quad (2.4)$$

and so on, and where $\delta_{\rho\sigma}$ is the Kronecker delta function and $\epsilon_{\rho\sigma\eta}$ is the Levi-Civita symbol, a totally antisymmetric tensor. Throughout this paper the Greek indices stand for three spatial directions (i.e., ρ, σ , etc. = 1, 2, 3) and we adopt the Einstein summation convention for repeated Greek indices.

If we denote the matrix in front of \vec{r} on the left-hand side of (2.2) by $D_{\rho\sigma}(\omega)$ and then solve for its inverse matrix, we get

$$\tilde{r}_{\rho}(\omega) = \alpha_{\rho\sigma}(\omega) [\tilde{f}_{\sigma}(\omega) + \tilde{F}_{\sigma}(\omega)] , \quad (2.5)$$

where

$$\alpha_{\rho\sigma}(\omega) \equiv [D(\omega)^{-1}]_{\rho\sigma} = \left[\lambda^2 \delta_{\rho\sigma} - \left(\omega \frac{e}{c} \right)^2 B_\rho B_\sigma - \epsilon_{\rho\sigma\eta} B_\eta \lambda i \omega \frac{e}{c} \right] / \det D(\omega), \quad (2.6)$$

with

$$\det D(\omega) = \lambda \left[\lambda^2 - \left(\omega \frac{e}{c} \right)^2 \bar{B}^2 \right] \quad (2.7)$$

and

$$\lambda(\omega) = -m\omega^2 + K - i\omega\bar{\mu}(\omega) \equiv [\alpha^{(0)}(\omega)]^{-1}. \quad (2.8)$$

Using the fact that $\bar{\mu}(\omega)^* = \bar{\mu}(-\omega)$, we deduce that $\alpha_{\rho\sigma}(\omega)$ given by (2.6) has the following properties:

$$\alpha_{\rho\sigma}(-\omega) = \alpha_{\rho\sigma}^*(\omega), \quad (2.9)$$

$$\alpha_{\rho\sigma}(\omega, \bar{B}) = \alpha_{\sigma\rho}(\omega, -\bar{B}). \quad (2.10)$$

Now let us introduce the position autocorrelation functions

$$\psi_{\rho\sigma}(t) \equiv \frac{1}{2} \langle r_\rho(t) r_\sigma(0) + r_\sigma(0) r_\rho(t) \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \tilde{\psi}_{\rho\sigma}(\omega). \quad (2.11)$$

Then, in the case of weak external forces (linear response theory), the Fourier transform $\tilde{\psi}_{\rho\sigma}(\omega)$ is related to $\alpha_{\rho\sigma}(\omega)$ by the fluctuation-dissipation theorem [see (A14) of Ref. 88]

$$\tilde{\psi}_{\rho\sigma}(\omega) = \frac{\hbar}{2i} \coth\left(\frac{\hbar\omega}{2kT}\right) [\alpha_{\rho\sigma}(\omega + i0^+) - \alpha_{\sigma\rho}^*(\omega + i0^+)]. \quad (2.12)$$

From (2.6), one can decompose $\alpha_{\rho\sigma}(\omega)$ into symmetric and antisymmetric parts:

$$\alpha_{\rho\sigma}(\omega) = \alpha_{\rho\sigma}^s(\omega) + \alpha_{\rho\sigma}^a(\omega) , \quad (2.13)$$

with

$$\alpha_{\rho\sigma}^s(\omega) = \left[\lambda^2 \delta_{\rho\sigma} - \left(\omega \frac{e}{c} \right)^2 B_\rho B_\sigma \right] / \det D(\omega) \quad (2.14)$$

and

$$\alpha_{\rho\sigma}^a(\omega) = \left(-\epsilon_{\rho\sigma\eta} B_\eta \lambda i \omega \frac{e}{c} \right) / \det D(\omega) . \quad (2.15)$$

Thus

$$\begin{aligned} \alpha_{\rho\sigma}(\omega) - \alpha_{\sigma\rho}^*(\omega) &= [\alpha_{\rho\sigma}^s(\omega) - \alpha_{\rho\sigma}^s(\omega)^*] + [\alpha_{\rho\sigma}^a(\omega) + \alpha_{\rho\sigma}^a(\omega)^*] \\ &= 2i \operatorname{Im} \alpha_{\rho\sigma}^s(\omega) + 2 \operatorname{Re} \alpha_{\rho\sigma}^a(\omega) . \end{aligned} \quad (2.16)$$

Combining (2.11), (2.12), and (2.16), and noting that $\operatorname{Im} \alpha_{\rho\sigma}^s(\omega)$ is an odd function of ω while $\operatorname{Re} \alpha_{\rho\sigma}^a(\omega)$ is an even function of ω , we have, finally,

$$\begin{aligned} \frac{1}{2} \langle r_\rho(t) r_\sigma(t') + r_\sigma(t') r_\rho(t) \rangle &= \frac{\hbar}{\pi} \int_0^\infty d\omega \operatorname{Im} [\alpha_{\rho\sigma}^s(\omega + i0^+)] \coth\left(\frac{\hbar\omega}{2kT}\right) \cos[\omega(t-t')] \\ &\quad - \frac{\hbar}{\pi} \int_0^\infty d\omega \operatorname{Re} [\alpha_{\rho\sigma}^a(\omega + i0^+)] \coth\left(\frac{\hbar\omega}{2kT}\right) \sin[\omega(t-t')] . \end{aligned} \quad (2.17)$$

III. Free Energy of the Oscillator

The Hamiltonian leading to (2.1) in the case where $\tilde{f}(t)$ is zero is

$$H_0 = \frac{1}{2m} \left[\bar{p} - \frac{e}{c} \bar{A} \right]^2 + \frac{1}{2} K \bar{r}^2 + \sum_j \left[\frac{\bar{p}_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 (\bar{q}_j - \bar{r})^2 \right] . \quad (3.1)$$

This is the independent-oscillator (IO) model in the presence of an external magnetic field \vec{B} , considered in an earlier paper [152], where e , m , \vec{r} , and \vec{p} are the charge, mass, position, and momentum of the oscillator, respectively; and the corresponding quantities with the lower indices j refer to the j th heat-bath oscillator. The vector potential \vec{A} is related to the magnetic field \vec{B} through the equation

$$\vec{B}(\vec{r}) = \vec{\nabla} \times \vec{A}(\vec{r}) . \quad (3.2)$$

To calculate the mean energy $\langle H_0 \rangle$ by the fluctuation–dissipation theorem, we are led, following Ford, Lewis, and O’Connell [88], to consider the Hamiltonian

$$H = H_0 - \vec{r} \cdot \vec{f}(t) - \sum_j \vec{q}_j \cdot \vec{f}_j(t) , \quad (3.3)$$

where $\vec{f}(t)$ and $\vec{f}_j(t)$ are c-number functions of time.

The Heisenberg equations of motion for the charged oscillator from (3.3) are

$$\dot{\vec{r}} = [\vec{r}, H]/i\hbar = \left[\vec{p} - \frac{e}{c} \vec{A} \right] / m , \quad (3.4)$$

$$\begin{aligned} \dot{\vec{p}} = [\vec{p}, H]/i\hbar = & -K\vec{r} + \sum_j m_j \omega_j^2 (\vec{q}_j - \vec{r}) + \frac{e}{c} (\dot{\vec{r}} \times \vec{B}) \\ & + \frac{e}{c} (\dot{\vec{r}} \cdot \vec{\nabla}) \vec{A} + \frac{i\hbar e}{2mc} \vec{\nabla} (\vec{\nabla} \cdot \vec{A}) + \vec{f} . \end{aligned} \quad (3.5)$$

For the heat-bath oscillators

$$\dot{\vec{q}}_j = [\vec{q}_j, H]/i\hbar = \vec{p}_j / m_j , \quad (3.6)$$

$$\dot{\vec{p}}_j = [\vec{p}_j, H]/i\hbar = -m_j \omega_j^2 (\vec{q}_j - \vec{r}) + \vec{f}_j . \quad (3.7)$$

Eliminating the momentum variables, (3.4) and (3.5) combine to give

$$m\ddot{\vec{r}} = -K\vec{r} + \sum_j m_j \omega_j^2 (\vec{q}_j - \vec{r}) + \frac{e}{c} (\dot{\vec{r}} \times \vec{B}) + \vec{f} . \quad (3.8)$$

Similarly, (3.6) and (3.7) yield

$$m_j \ddot{\tilde{q}}_j = -m_j \omega_j^2 \tilde{q}_j + m_j \omega_j^2 \tilde{r} + \tilde{f}_j . \quad (3.9)$$

For a detailed derivation of the Lorentz-force term $(e/c)(\dot{\tilde{r}} \times \tilde{B})$ in (3.8) we refer to Eqs. (7)–(15) of Ref. 152. Note that without \tilde{f} and \tilde{f}_j , (3.8) and (3.9) are just Eqs. (15) and (5) of Ref. 152, respectively. Using (3.4) and (3.6), and rearranging some terms, (3.1) can be written in the form

$$H_0 = \left[\frac{1}{2} m \dot{\tilde{r}}^2 + \frac{1}{2} \left(K + \sum_j m_j \omega_j^2 \right) \tilde{r}^2 \right] + \sum_j \left(\frac{1}{2} m_j \dot{\tilde{q}}_j^2 + \frac{1}{2} m_j \omega_j^2 \tilde{q}_j^2 \right) - \sum_j m_j \omega_j^2 \tilde{q}_j \cdot \tilde{r} . \quad (3.10)$$

We now turn to an evaluation of the ensemble average of H_0 , which is the mean energy of the system of the oscillator interacting with the heat bath in thermal equilibrium at temperature T . First, taking Fourier transforms, (3.8) and (3.9) become

$$\left[\delta_{\rho\sigma} \left(-m\omega^2 + K + \sum_j m_j \omega_j^2 \right) + i\omega \frac{e}{c} \varepsilon_{\rho\sigma\eta} B_\eta \right] \tilde{r}_\sigma - \sum_j m_j \omega_j^2 \tilde{q}_{j\rho} = \tilde{f}_\rho , \quad (3.11)$$

$$m_j (-\omega^2 + \omega_j^2) \tilde{q}_{j\rho} - m_j \omega_j^2 \tilde{r}_\rho = \tilde{f}_{j\rho} . \quad (3.12)$$

The solutions of these equations are

$$\tilde{r}_\rho = \alpha_{\rho\sigma} \tilde{f}_\sigma + \sum_j \beta_{j,\rho\sigma} \tilde{f}_{j\sigma} , \quad (3.13)$$

$$\tilde{q}_{j\rho} = \beta_{j,\rho\sigma} \tilde{f}_\sigma + \sum_i \gamma_{ji,\rho\sigma} \tilde{f}_{i\sigma} , \quad (3.14)$$

where $\alpha_{\rho\sigma}(\omega)$, the oscillator susceptibility, is given by (2.6),

$$\beta_{j,\rho\sigma}(\omega) \equiv \frac{\omega_j^2}{-\omega^2 + \omega_j^2} \alpha_{\rho\sigma}(\omega) \quad (3.15)$$

is the cross susceptibility, and

$$\gamma_{ji,\rho\sigma}(\omega) \equiv \frac{\omega_i^2 \omega_j^2}{(\omega^2 - \omega_i^2)(\omega^2 - \omega_j^2)} \alpha_{\rho\sigma}(\omega) + \frac{\delta_{ij} \delta_{\rho\sigma}}{m_j(-\omega^2 + \omega_j^2)} \quad (3.16)$$

is the heat-bath oscillator susceptibility. Since $\alpha_{\rho\sigma}^a(\omega) = 0$ if $\rho = \sigma$, from (2.17) we immediately get

$$\frac{1}{2} \langle \bar{r}(t) \cdot \bar{r}(t') + \bar{r}(t') \cdot \bar{r}(t) \rangle = \frac{\hbar}{\pi} \int_0^\infty d\omega \operatorname{Im} [\alpha_{\rho\rho}(\omega + i0^+)] \coth\left(\frac{\hbar\omega}{2kT}\right) \cos[\omega(t - t')], \quad (3.17)$$

which, of course, is a special case of (2.17). Differentiating with respect to t and t' and then setting t' equal to t , we have

$$\langle \dot{\bar{r}}^2 \rangle = \frac{\hbar}{\pi} \int_0^\infty d\omega \coth\left(\frac{\hbar\omega}{2kT}\right) \operatorname{Im} [\alpha_{\rho\rho}(\omega + i0^+)] \omega^2. \quad (3.18)$$

Similar expressions hold for $\langle \bar{q}_j^2 \rangle$ and $\langle \dot{\bar{q}}_j^2 \rangle$, with $\alpha_{\rho\rho}$ being replaced by $\gamma_{jj,\rho\rho}$ in (3.17) and (3.18). For $\langle \bar{q}_j \cdot \bar{r} \rangle$, noting the symmetry of the cross susceptibility $\beta_{j,\rho\sigma}$ in (3.13) and (3.14), we have a similar result with $\beta_{j,\rho\rho}$ replacing $\alpha_{\rho\rho}$:

$$\langle \bar{q}_j \cdot \bar{r} \rangle = \frac{\hbar}{\pi} \int_0^\infty d\omega \coth\left(\frac{\hbar\omega}{2kT}\right) \operatorname{Im} [\beta_{j,\rho\rho}(\omega + i0^+)]. \quad (3.19)$$

The second group of terms in (3.10) is the Hamiltonian of the heat bath in the absence of the oscillator. We denote it as H_B . Its mean value is given by

$$\begin{aligned}
\langle H_B \rangle &= \sum_j \frac{\hbar}{\pi} \int_0^\infty d\omega \coth\left(\frac{\hbar\omega}{2kT}\right) \frac{1}{2} m_j (\omega^2 + \omega_j^2) \text{Im} \left[\gamma_{jj,\rho\rho}(\omega + i0^+) \right] \\
&= \frac{\hbar}{2\pi} \int_0^\infty d\omega \coth\left(\frac{\hbar\omega}{2kT}\right) \text{Im} \left\{ \sum_j m_j (\omega^2 + \omega_j^2) \left[\frac{\omega_j^4}{(\omega^2 - \omega_j^2)^2} \alpha_{\rho\rho} + \frac{3}{m_j(-\omega^2 + \omega_j^2)} \right] \right\} \\
&= \frac{\hbar}{2\pi} \int_0^\infty d\omega \coth\left(\frac{\hbar\omega}{2kT}\right) \text{Im} \left[\sum_j \frac{m_j (\omega^2 + \omega_j^2) \omega_j^4}{(\omega^2 - \omega_j^2)^2} \alpha_{\rho\rho} \right] \\
&\quad + \frac{\hbar}{2\pi} \sum_j \int_0^\infty d\omega \coth\left(\frac{\hbar\omega}{2kT}\right) \text{Im} \left\{ \frac{3(\omega^2 + \omega_j^2)}{\omega + \omega_j} \left[P\left(\frac{1}{\omega_j - \omega}\right) + i\pi\delta(\omega_j - \omega) \right] \right\} \\
&= \frac{\hbar}{2\pi} \int_0^\infty d\omega \coth\left(\frac{\hbar\omega}{2kT}\right) \text{Im} \left[\sum_j \frac{m_j (\omega^2 + \omega_j^2) \omega_j^4}{(\omega^2 - \omega_j^2)^2} \alpha_{\rho\rho} \right] + 3 \sum_j \frac{\hbar\omega_j}{2} \coth\left(\frac{\hbar\omega_j}{2kT}\right).
\end{aligned} \tag{3.20}$$

In the second line above, we have used (3.16) to calculate the trace $\gamma_{jj,\rho\rho}$, while the fourth line follows from the identity

$$\frac{1}{\omega - \omega_j + i0^+} = P\left(\frac{1}{\omega - \omega_j}\right) - i\pi\delta(\omega - \omega_j), \tag{3.21}$$

where P denotes the principal value. (Remember that ω in the integral is approached from above the real axis, i.e., $\omega \rightarrow \omega + i0^+$.) The last term of (3.20) is readily recognized as the mean energy of the free heat bath in the absence of the oscillator, which we shall denote as $U_B(T)$, as in Ref. 88.

Combining the results (3.17)–(3.20) and using (3.10), we find the oscillator energy, which is defined as the mean energy of the system of the oscillator interacting with the heat bath minus the mean energy of the heat bath in the absence of the oscillator:

$$\begin{aligned}
U_O(T, B) &\equiv \langle H_0 \rangle - U_B(T) = \frac{\hbar}{\pi} \int_0^\infty d\omega \coth\left(\frac{\hbar\omega}{2kT}\right) \left\{ \text{Im}(\alpha_{\rho\rho}) \frac{1}{2} \left(m\omega^2 + K + \sum_j m_j \omega_j^2 \right) \right. \\
&\quad \left. + \frac{1}{2} \sum_j \text{Im} \left[\frac{m_j (\omega^2 + \omega_j^2) \omega_j^4}{(\omega^2 - \omega_j^2)^2} \alpha_{\rho\rho} \right] - \sum_j m_j \omega_j^2 \text{Im}(\beta_{j,\rho\rho}) \right\} \\
&= \frac{\hbar}{2\pi} \int_0^\infty d\omega \coth\left(\frac{\hbar\omega}{2kT}\right) \text{Im} \left\{ \alpha_{\rho\rho} \left[m\omega^2 + K + \sum_j \frac{\omega^2 + \omega_j^2}{(\omega^2 - \omega_j^2)^2} \omega^2 m_j \omega_j^2 \right] \right\}.
\end{aligned} \tag{3.22}$$

The last equation follows from (3.15).

Since the memory function of the heat bath associated with the Hamiltonian (3.1) is [88]

$$\tilde{\mu}(\omega) = \frac{i}{2} \sum_j m_j \omega_j^2 \left(\frac{1}{\omega - \omega_j} + \frac{1}{\omega + \omega_j} \right), \tag{3.23}$$

thus

$$\frac{d}{d\omega} \tilde{\mu}(\omega) = -i \sum_j m_j \omega_j^2 \frac{\omega^2 + \omega_j^2}{(\omega^2 - \omega_j^2)^2}. \tag{3.24}$$

Substituting (3.24) into (3.22), we have

$$U_O(T, B) = \frac{\hbar}{2\pi} \int_0^\infty d\omega \coth\left(\frac{\hbar\omega}{2kT}\right) \text{Im} \left[\alpha_{\rho\rho}(\omega) \left(m\omega^2 + K + i\omega^2 \frac{d}{d\omega} \tilde{\mu}(\omega) \right) \right]. \tag{3.25}$$

This equation can be simplified further. From (2.6), the trace of $\alpha_{\rho\sigma}(\omega)$ is

$$\alpha_{\rho\rho}(\omega) = \left[3\lambda^2 - \left(\omega \frac{e}{c} \right)^2 \bar{B}^2 \right] / \det D(\omega) \tag{3.26}$$

and, from (2.6) and (2.7), the determinant of $\alpha_{\rho\sigma}(\omega)$ is

$$\det \alpha(\omega) = [\det D(\omega)]^{-1} = \left\{ \lambda \left[\lambda^2 - \left(\omega \frac{e}{c} \right)^2 \bar{B}^2 \right] \right\}^{-1}, \quad (3.27)$$

where [rewriting (2.8) for convenience]

$$\lambda(\omega) = [\alpha^{(0)}(\omega)]^{-1} = -m\omega^2 + K - i\omega\tilde{\mu}(\omega). \quad (3.28)$$

Hence

$$\begin{aligned} \omega \frac{d}{d\omega} \{ \ln [\det \alpha(\omega)] \} &= -\omega \left\{ \frac{d\lambda}{d\omega} \left[3\lambda^2 - \left(\omega \frac{e}{c} \right)^2 \bar{B}^2 \right] - 2\omega\lambda \left(\frac{e}{c} \right)^2 \bar{B}^2 \right\} / \det D(\omega) \\ &= -3 + \left(\lambda - \omega \frac{d\lambda}{d\omega} \right) \left[3\lambda^2 - \left(\omega \frac{e}{c} \right)^2 \bar{B}^2 \right] / \det D(\omega) \\ &= -3 + \left(\lambda - \omega \frac{d\lambda}{d\omega} \right) \alpha_{\rho\rho}(\omega). \end{aligned} \quad (3.29)$$

By (3.28)

$$\lambda - \omega \frac{d\lambda}{d\omega} = m\omega^2 + K + i\omega^2 \frac{d}{d\omega} \tilde{\mu}(\omega). \quad (3.30)$$

Thus

$$\left[m\omega^2 + K + i\omega^2 \frac{d}{d\omega} \tilde{\mu}(\omega) \right] \alpha_{\rho\rho}(\omega) = 3 + \omega \frac{d}{d\omega} \{ \ln [\det(\omega)] \}. \quad (3.31)$$

Substituting (3.31) in (3.25), we finally obtain

$$U_O(T, B) = \frac{1}{\pi} \int_0^\infty d\omega u(\omega, T) \operatorname{Im} \left\{ \frac{d}{d\omega} \ln [\det \alpha(\omega + i0^+)] \right\}, \quad (3.32)$$

where $u(\omega, T)$ is the Planck energy (including zero-point energy) of a free oscillator of frequency ω :

$$u(\omega, T) = \frac{\hbar\omega}{2} \coth \left(\frac{\hbar\omega}{2kT} \right), \quad (3.33)$$

and $\det \alpha(\omega)$ is given by (3.27) and (3.28). The corresponding formula for the free energy of the oscillator takes the form

$$F_O(T, B) = \frac{1}{\pi} \int_0^\infty d\omega f(\omega, T) \operatorname{Im} \left\{ \frac{d}{d\omega} \ln [\det \alpha(\omega + i0^+)] \right\}, \quad (3.34)$$

where $f(\omega, T)$ is the free energy (including zero-point energy) of a free oscillator of frequency ω :

$$f(\omega, T) = kT \ln [2 \sinh(\hbar \omega / 2kT)]. \quad (3.35)$$

Equations (3.32) and (3.34) represent extensions, to $B \neq 0$, of the "remarkable formulas" given in Ref. 83 for the case $B = 0$. It will be noticed that the corresponding results in Ref. 83 [see also (1.2) above] have $\alpha^{(0)}(\omega)$, the scalar susceptibility in the absence of a magnetic field, instead of $\det \alpha(\omega)$. To make the role of the magnetic field more explicit, we now use (3.27) and (3.28) to write

$$\det \alpha(\omega) = [\alpha^{(0)}(\omega)]^3 \left[1 - \left(\frac{eB\omega}{c} \right)^2 [\alpha^{(0)}(\omega)]^2 \right]^{-1} \quad (3.36)$$

so that

$$F_O(T, B) = F_O(T, 0) + \Delta F_O(T, B), \quad (3.37)$$

where

$$F_O(T, 0) = \frac{3}{\pi} \int_0^\infty d\omega f(\omega, T) \operatorname{Im} \left[\frac{d}{d\omega} \ln \alpha^{(0)}(\omega) \right] \quad (3.38)$$

is the free energy of the oscillator in the absence of the magnetic field [in agreement with Eq. (5) of Ref. 83, except for the extra factor of 3 which results from our consideration here of three dimensions] and the correction due to the magnetic field is given by

$$\Delta F_O(T, B) = -\frac{1}{\pi} \int_0^\infty d\omega f(\omega, T) \operatorname{Im} \left\{ \frac{d}{d\omega} \ln \left[1 - \left(\frac{eB\omega}{c} \right)^2 [\alpha^{(0)}(\omega)]^2 \right] \right\}, \quad (3.39)$$

where $\alpha^{(0)}(\omega)$ is defined in (2.8). Our basic result (3.34) may also be derived (see the Appendix) using a succinct (but perhaps a less transparent) method, which is a natural generalization of the method given in Ref. 83 for the $B = 0$ situation.

IV. Ohmic and Blackbody Radiation Heat Baths

In this section, we will apply the formulas derived in Sec. III to two types of heat baths.

A. Ohmic heat bath

In the case of the Ohmic heat bath, $\tilde{\mu}(\omega) = m\gamma$, a constant, which is the simplest memory function one can choose. Thus making use of (3.27) and (3.28), (3.34) becomes

$$F_O(T, B) = \frac{1}{\pi} \int_0^\infty d\omega f(\omega, T) \left[\frac{\gamma(\omega^2 + \omega_0^2)}{(\omega^2 - \omega_0^2)^2 + \gamma^2 \omega^2} + \frac{\gamma(\omega^2 + \omega_0^2)}{(\omega^2 - \omega_0^2 + \omega_c \omega)^2 + \gamma^2 \omega^2} + \frac{\gamma(\omega^2 + \omega_0^2)}{(\omega^2 - \omega_0^2 - \omega_c \omega)^2 + \gamma^2 \omega^2} \right], \quad (4.1)$$

where $\omega_0 = (K/m)^{1/2}$ is the bare-oscillator frequency and $\omega_c = eB/mc$ is the cyclotron frequency. For the internal energy $U_O(T, B)$, we see from a comparison of (3.32) and (3.34) that one need only replace $f(\omega, T)$ in (4.1) by $u(\omega, T)$, which is given by (3.33).

In the high-temperature limit

$$u(\omega, T) = \frac{\hbar\omega}{2} \coth\left(\frac{\hbar\omega}{2kT}\right) \rightarrow kT, \quad (4.2)$$

and, using the method of contour integration, one can show that

$$\begin{aligned}
U_O(T, B) &= \frac{kT}{\pi} \int_0^\infty d\omega \left[\frac{\gamma(\omega^2 + \omega_0^2)}{(\omega^2 - \omega_0^2)^2 + \gamma^2 \omega^2} + \frac{\gamma(\omega^2 + \omega_0^2)}{(\omega^2 - \omega_0^2 + \omega_c \omega)^2 + \gamma^2 \omega^2} \right. \\
&\quad \left. + \frac{\gamma(\omega^2 + \omega_0^2)}{(\omega^2 - \omega_0^2 - \omega_c \omega)^2 + \gamma^2 \omega^2} \right] \\
&= \begin{cases} 3kT & \text{if } \omega_0 \neq 0 \\ \frac{3}{2}kT & \text{if } \omega_0 = 0. \end{cases} \quad (4.3)
\end{aligned}$$

This is classical result, which we note is independent of B .

At $T = 0$ K, $f(\omega, T) = u(\omega, T) \rightarrow \hbar\omega/2$ and thus both $F_O(0, B)$ and $U_O(0, B)$ are logarithmically divergent. That is due to the contribution of the zero-point energy, which is of no physical significance since it is not directly observable. However, the difference $\Delta F_O(0, B) = F_O(0, B) - F_O(0, B=0)$ is finite. From (3.39), we have

$$\begin{aligned}
\Delta F_O(0, B) &= \frac{\hbar}{2\pi} \int_0^\infty d\omega \omega \left[\frac{\gamma(\omega^2 + \omega_0^2)}{(\omega^2 - \omega_0^2 + \omega_c \omega)^2 + \gamma^2 \omega^2} \right. \\
&\quad \left. + \frac{\gamma(\omega^2 + \omega_0^2)}{(\omega^2 - \omega_0^2 - \omega_c \omega)^2 + \gamma^2 \omega^2} - \frac{2\gamma(\omega^2 + \omega_0^2)}{(\omega^2 - \omega_0^2)^2 + \gamma^2 \omega^2} \right], \quad (4.4)
\end{aligned}$$

which is a function of ω_c^2 . This integral can be expressed in closed form:

$$\begin{aligned}
\Delta F_O(0, B) &= \frac{\hbar}{\pi} \left\{ 2 \left(\frac{b+a}{2} \right)^{1/2} \tan^{-1} \left[\frac{2 \left(\frac{b+a}{2} \right)^{1/2}}{\gamma} \right] - \left(\frac{b-a}{2} \right)^{1/2} \ln \left[\frac{\gamma/2 + \sqrt{(b-a)/2}}{\gamma/2 - \sqrt{(b-a)/2}} \right] \right. \\
&\quad \left. - 2 \left(\omega_0^2 - \frac{1}{4} \gamma^2 \right)^{1/2} \tan^{-1} \left[\frac{2 \left(\omega_0^2 - \frac{1}{4} \gamma^2 \right)^{1/2}}{\gamma} \right] \right\}, \quad (4.5)
\end{aligned}$$

where

$$b = \left\{ \left[\left(\frac{\omega_c}{2} \right)^2 + \left(\omega_0 + \frac{\gamma}{2} \right)^2 \right] \left[\left(\frac{\omega_c}{2} \right)^2 + \left(\omega_0 - \frac{\gamma}{2} \right)^2 \right] \right\}^{1/2}$$

and

$$a = \left(\frac{\omega_c}{2} \right)^2 + \omega_0^2 - \frac{\gamma^2}{4} . \quad (4.6)$$

Taking the derivative of $\Delta F_O(0, B)$ with respect to $(\omega_c/2)^2$ (denoted by z), we get

$$\begin{aligned} \frac{d}{dz} \Delta F_O(0, B) = \frac{\hbar}{\pi b} \left\{ \frac{\gamma^2/4 + [(b+a)/2]}{\sqrt{(b+a)/2}} \tan^{-1} \left[\frac{2}{\gamma} \left(\frac{b+a}{2} \right)^{1/2} \right] \right. \\ \left. - \frac{\gamma^2/4 - [(b-a)/2]}{2\sqrt{(b-a)/2}} \ln \left[\frac{\gamma/2 + \sqrt{(b-a)/2}}{\gamma/2 - \sqrt{(b-a)/2}} \right] \right\} . \end{aligned} \quad (4.7)$$

By virtue of the inequalities $(1/2) \ln[(1+x)/(1-x)] < x/(1-x^2)$ ($0 < x < 1$) and $\tan^{-1} x > x/(1+x^2)$ ($x > 0$), one can show that

$$\frac{\gamma^2/4 + [(b+a)/2]}{\sqrt{(b+a)/2}} \tan^{-1} \left[\frac{2}{\gamma} \left(\frac{b+a}{2} \right)^{1/2} \right] > \frac{\gamma}{2} \quad (4.8)$$

and

$$\frac{\gamma^2/4 - [(b-a)/2]}{2\sqrt{(b-a)/2}} \ln \left[\frac{\gamma/2 + \sqrt{(b-a)/2}}{\gamma/2 - \sqrt{(b-a)/2}} \right] < \frac{\gamma}{2} . \quad (4.9)$$

Hence

$$\frac{d}{dz} \Delta F_O(0, B) > 0 , \quad (4.10)$$

which means that $\Delta F_O(0, B)$ is a monotonically increasing function of ω_c^2 . This diamagnetic behavior is what we would expect from the orbital origin of the magnetism (since spin has been neglected).

In the weak-field limit ($B \rightarrow 0$), (4.5) can be expanded as a series of ω_c^2 :

$$\Delta F_O(0, B) = \begin{cases} \frac{\hbar}{2\pi\gamma} \left(\frac{\chi^2 + 1}{\chi^3} \tan^{-1} \chi - \frac{1}{\chi^2} \right) \omega_c^2 & \text{if } \omega_c^2 \ll \left| \omega_0^2 - \frac{\gamma^2}{4} \right| \\ \frac{\hbar}{3\pi\gamma} \omega_c^2 & \text{if } \omega_0 = \frac{\gamma}{2}, \end{cases} \quad (4.11)$$

where $\chi \equiv (2/\gamma)(\omega_0^2 - \gamma^2/4)^{1/2}$. The omitted terms in Eq. (4.11) are of the order of ω_c^4 .

In both (4.5) and (4.11), $2(\omega_0^2 - \gamma^2/4)^{1/2} \tan^{-1} \left[(2/\gamma)(\omega_0^2 - \gamma^2/4)^{1/2} \right]$ should be replaced by

$$-(\gamma^2/4 - \omega_0^2)^{1/2} \ln \left[\frac{\gamma/2 + (\gamma^2/4 - \omega_0^2)^{1/2}}{\gamma/2 - (\gamma^2/4 - \omega_0^2)^{1/2}} \right]$$

when $\omega_0 < \gamma/2$. This is due to the identity $\tan^{-1}(ix) = (i/2) \ln[(1+x)/(1-x)]$.

We note that the coefficients in front of ω_c^2 in (4.11) are positive because of the inequalities in (4.8) with $\omega_c = 0$. As a final comment, we note that no mass renormalization is necessary, in contrast to what we will find in the next example.

B. Blackbody radiation heat bath

In this case, the associated memory function is [83]

$$\tilde{\mu}(\omega) = 2e^2 \Omega^2 \omega / 3c^3 (\omega + i\Omega), \quad (4.12)$$

where Ω is a large cutoff frequency.

Thus

$$\begin{aligned} \lambda \pm \frac{eB\omega}{c} &= -m\omega^2 + K - i\omega\tilde{\mu}(\omega) \pm \frac{eB\omega}{c} \\ &= \frac{m}{\omega + i\Omega} \left[-\omega^3 - \left(i\frac{M\Omega}{m} \mp \frac{eB}{mc} \right) \omega^2 \pm \left(i\frac{eB}{mc} \Omega \pm \frac{K}{m} \right) \omega + i\frac{K\Omega}{m} \right], \end{aligned} \quad (4.13)$$

where

$$M = m + 2e^2\Omega/3c^3 \quad (4.14)$$

is the renormalized mass. In the limit of large cutoff ($\Omega \rightarrow 1/\tau_e$ or, equivalently, $m \rightarrow 0$), the numerator in (4.13) can be factored to give

$$\lambda \pm \frac{eB\omega}{c} = \frac{m}{\omega + i\Omega} \left(\omega + i\frac{M\Omega}{m} \right) \left[-\omega^2 + \omega_0^2 \mp i\omega_c\tau_e\omega_0^2 - i(\omega_0^2 + \omega_c^2)\tau_e\omega \pm \omega_c\omega \right], \quad (4.15)$$

where $\omega_0^2 = K/M$, $\omega_c = eB/Mc$, and $\tau_e \equiv 2e^2/3Mc^3 \equiv 6.27 \times 10^{-24}$ s for the electron. Because $\omega_c = 1.76 \times 10^{11} (B/10^4 \text{ G}) \text{ Hz}$ and the atomic unit of frequency is $4 \times 10^{15} \text{ Hz}$, we see that typically

$$\omega_c\tau_e \ll 1. \quad (4.16)$$

Also, if we assume that $\omega_c \ll \omega_0$, then (4.15) can be simplified to

$$\lambda \pm \frac{eB\omega}{c} = \frac{M}{1 - i\tau_e\omega} \left(-\omega^2 + \omega_0^2 - i\omega_0^2\tau_e\omega \pm \omega_c\omega \right). \quad (4.17)$$

Thus

$$\begin{aligned} \det \alpha(\omega) &= \frac{1}{\lambda \left[\lambda^2 - (e/c)^2 B^2 \omega^2 \right]} \\ &= \frac{1 - i\tau_e\omega}{M(-\omega^2 + \omega_0^2 - i\omega_0^2\tau_e\omega)} \times \frac{1 - i\tau_e\omega}{M(-\omega^2 + \omega_0^2 - i\omega_0^2\tau_e\omega + \omega_c\omega)} \\ &\quad \times \frac{1 - i\tau_e\omega}{M(-\omega^2 + \omega_0^2 - i\omega_0^2\tau_e\omega - \omega_c\omega)}. \end{aligned} \quad (4.18)$$

Substituting (4.18) into (3.34) and using (4.16), as well as the fact that $\hbar\tau_e^{-1} \gg kT$, we obtain the expression for the oscillator free energy

$$F_O(T, B) = \frac{1}{\pi} \int_0^\infty d\omega f(\omega, T) \left[\frac{\gamma(\omega^2 + \omega_0^2)}{(\omega^2 - \omega_0^2)^2 + \gamma^2 \omega^2} + \frac{\gamma(\omega^2 + \omega_0^2)}{(\omega^2 - \omega_0^2 + \omega_c \omega)^2 + \gamma^2 \omega^2} \right. \\ \left. + \frac{\gamma(\omega^2 + \omega_0^2)}{(\omega^2 - \omega_0^2 - \omega_c \omega)^2 + \gamma^2 \omega^2} \right] + \frac{\pi e^2 (kT)^2}{3\hbar M c^3}, \quad (4.19)$$

where $\gamma = \omega_0^2 \tau_e$. The first term corresponds to the result given in (4.1) for the case of $\tilde{\mu}(\omega) = m\gamma$. The second term is the familiar temperature-dependent shift [83], which is independent of the magnetic field.

V. Absence of a Heat Bath

The limit of no dissipation (no heat bath) is simply obtained by taking $\tilde{\mu}(\omega) = 0$. Thus writing $K \equiv m\omega_0^2$, we see from (3.28) that

$$\lambda(\omega) = [\alpha^{(0)}(\omega)]^{-1} \rightarrow -m(\omega^2 - \omega_0^2) \quad (5.1)$$

and

$$\left[1 - \left(\frac{eB\omega}{c} \right)^2 [\alpha^{(0)}(\omega)]^2 \right] \rightarrow \frac{1}{(\omega^2 - \omega_0^2)^2} [(\omega^2 - \omega_0^2)^2 - (\omega_c \omega)^2], \quad (5.2)$$

where

$$\omega_c \equiv eB/mc \quad (5.3)$$

is the cyclotron frequency. These results, when substituted into (3.38) and (3.39), lead to

$$F_O(T, 0) = 3f(\omega_0, T) \quad (5.4)$$

and

$$\Delta F_O(T, B) = f(\omega_1, T) + f(\omega_2, T) - 2f(\omega_0, T), \quad (5.5)$$

where

$$\omega_{1,2} = \pm(\omega_c/2) + \left[(\omega_c/2)^2 + \omega_0^2 \right]^{1/2}, \quad (5.6)$$

and $f(\omega, T)$ is given by (3.35). Hence, from (3.37),

$$F_O(T, B) = \sum_{i=0,1,2} f(\omega_i, T). \quad (5.7)$$

Similarly,

$$U_O(T, B) = \sum_{i=0,1,2} u(\omega_i, T), \quad (5.8)$$

where $u(\omega, T)$ is given by (3.33). It immediately follows that the eigenspectrum of a charged oscillator in a magnetic field is given by

$$E = \sum_{i=0,1,2} \hbar \omega_i \left(n_i + \frac{1}{2} \right) \quad \text{where } n_i = 0, 1, 2, \dots \quad (5.9)$$

This is a well-known result [163], but it is interesting that we have obtained it in a rather novel fashion as a special case of our general formalism.

In fact, an even simpler derivation of (5.9) follows from the fact (see the Appendix) that the poles of $\alpha(\omega)$ occur for ω values equal to the normal-mode frequencies of the interacting system ($\bar{\omega}_j$ say). Hence from (3.27), we have

$$\lambda(\bar{\omega}_j) \left[\lambda^2(\bar{\omega}_j) - (m\omega_c \bar{\omega}_j)^2 \right] = 0. \quad (5.10)$$

In the case where $\tilde{\mu}(\omega) = 0$, we have from (3.28) that

$$\lambda(\bar{\omega}_j) = m(\omega_0^2 - \bar{\omega}_j^2). \quad (5.11)$$

Thus Eqs. (5.10) and (5.11) imply $\bar{\omega}_j$ values equal to ω_0 , ω_1 , and ω_2 as before, so that Eqs. (5.7)–(5.9) again follow.

VI. Conclusions

We have shown that the problem of a charged oscillator moving in a harmonic potential well and a uniform external magnetic field, and coupled to an arbitrary physical heat bath can be solved exactly using the generalized quantum Langevin equation. The free energy (3.34) together with the explicit expression for $\det \alpha(\omega)$, given in (3.27) and (3.28), can in principle determine all the relevant quantities of the problem.

Appendix: Alternative Derivation of Eq. (3.34)

Our method is a generalization of the method given in Ref. 83 for the case of zero magnetic field. We start with Eq. (2.5) in the absence of an external field:

$$\tilde{r}_\rho(\omega) = \alpha_{\rho\sigma}(\omega) \tilde{F}_\sigma(\omega) . \quad (\text{A1})$$

Thus the necessary and sufficient condition that there be a fluctuating force in the absence of a displacement [$\tilde{r}(\omega) = 0$] is that

$$\det \alpha(\omega) = 0 . \quad (\text{A2})$$

It follows that the zeros of $\det \alpha(\omega)$ occur for ω values equal to the normal-mode frequencies of the radiation field in the absence of the oscillator (ω_i say). In a similar manner, we note that if we invert (A1) to write

$$\left[\alpha(\omega)^{-1} \right]_{\rho\sigma} \tilde{r}_\sigma(\omega) = \tilde{F}_\rho(\omega) , \quad (\text{A3})$$

then it follows that there can be a nonzero displacement with no force [$\tilde{F}_\sigma(\omega) = 0$] if

$$\det \alpha(\omega)^{-1} = 1/\det \alpha(\omega) = 0 . \quad (\text{A4})$$

Hence the poles of $\det \alpha(\omega)$ occur for ω values equal to the normal-mode frequencies of the interacting system ($\bar{\omega}_j$ say). Therefore one can write

$$\det \alpha(\omega) \propto \prod_i (\omega^2 - \omega_i^2) / \prod_j (\omega^2 - \bar{\omega}_j^2), \quad \text{Im } \omega > 0. \quad (\text{A5})$$

Now, recalling the identity

$$\frac{1}{x + i0^+} = \text{P} \left(\frac{1}{x} \right) - i\pi \delta(x), \quad (\text{A6})$$

we see that

$$\begin{aligned} & \pi^{-1} \text{Im} [d \ln \det \alpha(\omega) / d\omega] \\ &= \sum_j [\delta(\omega - \bar{\omega}_j) + \delta(\omega + \bar{\omega}_j)] - \sum_i [\delta(\omega - \omega_i) + \delta(\omega + \omega_i)]. \end{aligned} \quad (\text{A7})$$

When this is put into (3.34), the result can be written as

$$F_O(T) = \sum_j f(\bar{\omega}_j, T) - \sum_i f(\omega_i, T), \quad (\text{A8})$$

which is precisely the definition of the free energy of the oscillator, where the first sum on the right-hand side of (A8) is clearly the free energy of the interacting system and the second is that of the free field. This demonstrates the correctness of (3.34).

4. Dissipative Effects on the Localization of a Charged Oscillator in a Magnetic Field*

I. Introduction

The problem of dissipative effects on localization has been investigated by many people in connection with the study of dissipative quantum phase coherence [77,99,100 – 103,105]. It has been shown recently [125], by calculating explicitly the equal-time position autocorrelation functions for a specific model of a one-dimensional quantum harmonic oscillator in both Ohmic and blackbody radiation heat baths at arbitrary temperatures, that increasing dissipation always results in enhanced localization, in agreement

*This section consists of the body text of Ref. 157, by X. L. Li, G. W. Ford, and R. F. O'Connell, with its abstract incorporated in Sec. 1 (Introduction to Chapter III) and its references merged into the overall bibliography.

with previous work on the subject [77]. These results are not unexpected. Now we wish to extend these considerations to the case of an external field, specifically a magnetic field. We find that the interplay between the dissipation and the external field not only complicates the problem but also gives rise to unexpected results. In the following, we will extend our earlier work to that of a three-dimensional charged quantum oscillator in a heat bath and in the presence of a uniform magnetic field.

For simplicity, we shall restrict our consideration here to the case of an Ohmic heat bath at zero temperature. In Sec. II, we calculate in detail the equal-time position autocorrelation functions and their derivatives with respect to the frictional parameter of the Ohmic heat bath. In Sec. III, we summarize the analysis, give a physical interpretation of our results, and present our conclusions.

II. Position Autocorrelation Function

For a particle of charge e and mass m in a three-dimensional (3D) harmonic potential well with spring constant K , in the presence of a uniform static magnetic field \vec{B} , and coupled to a heat bath at zero temperature, the equal-time position autocorrelation functions can be derived using a generalized quantum Langevin equation (GLE) with the result [see Eq. (2.17) in Ref. 155 and set $T = 0$ and $t = t'$]

$$\frac{1}{2} \langle r_\rho r_\sigma + r_\sigma r_\rho \rangle = \frac{\hbar}{\pi} \int_0^\infty d\omega \operatorname{Im} \left[\alpha_{\rho\sigma}^s(\omega + i0^+) \right], \quad (2.1)$$

where the Greek indices ρ and σ stand for different spatial components of the position operator \vec{r} , and $\alpha_{\rho\sigma}^s(\omega)$ is the symmetric part of the generalized susceptibility tensor [Eqs. (2.14) and (3.28) of Ref. 155]. Explicitly,

$$\alpha_{\rho\sigma}^s(\omega) = \left[\lambda^2 \delta_{\rho\sigma} - \left(\omega \frac{e}{c} \right)^2 B_\rho B_\sigma \right] / \left\{ \lambda \left[\lambda^2 - \left(\omega \frac{e}{c} \right)^2 \bar{B}^2 \right] \right\} \quad (2.2)$$

and

$$\lambda(\omega) = -m\omega^2 + K - i\omega\tilde{\mu}(\omega), \quad (2.3)$$

where $\tilde{\mu}(\omega)$ is the spectral distribution of the heat bath [82]. For an Ohmic heat bath, it is frequency independent, i.e., $\tilde{\mu}(\omega) = m\gamma$, where γ is the so-called friction constant.

Without loss of generality, we assume that the magnetic field is along the z axis. Then the only nonzero components of $\alpha_{\rho\sigma}^s(\omega)$ are

$$\alpha_{xx}^s(\omega) = \alpha_{yy}^s(\omega) = \frac{\lambda}{\lambda^2 - (e/c)^2 \bar{B}^2 \omega^2} \quad (2.4)$$

and

$$\alpha_{zz}^s(\omega) = \frac{1}{\lambda} = \frac{1}{-m\omega^2 + K - i\omega\tilde{\mu}(\omega)}. \quad (2.5)$$

Correspondingly, the only nonzero position autocorrelation functions here are the mean square displacements $\langle x^2 \rangle$, $\langle y^2 \rangle$, and $\langle z^2 \rangle$.

We note here that $\alpha_{zz}^s(\omega)$ is the same as that for a one-dimensional problem without the magnetic field, and that it can be obtained formally by setting \bar{B} equal to zero in the expression (2.4) for α_{xx}^s or α_{yy}^s . Hence $\alpha_{zz}^s(\omega)$ and $\langle z^2 \rangle$ are independent of the magnetic field, which is expected because a magnetic field does not affect the motion of particles along the field line itself.

Using (2.3) and (2.4), and taking $\tilde{\mu}(\omega) = m\gamma$, it follows that

$$\begin{aligned} \text{Im } \alpha_{xx}^s(\omega) &= \frac{\gamma\omega}{2m} \left[\frac{1}{(\omega^2 - \omega_0^2 + \omega_c\omega)^2 + \gamma^2\omega^2} + \frac{1}{(\omega^2 - \omega_0^2 - \omega_c\omega)^2 + \gamma^2\omega^2} \right] \\ &= \frac{\omega}{2m} \text{Im} \left\{ \frac{1}{\sqrt{\Delta}} \left[\frac{1}{\omega^2 + \omega_2^2} - \frac{1}{\omega^2 + \omega_1^2} \right] \right\}, \end{aligned} \quad (2.6)$$

where $\omega_0 = (K/m)^{1/2}$ is the bare-oscillator frequency and $\omega_c \equiv eB/mc$ is the cyclotron frequency, while

$$\Delta = \left(\frac{\omega_c + i\gamma}{2} \right)^2 + \omega_0^2 \quad \text{and} \quad \omega_{1,2} = \frac{\gamma - i\omega_c}{2} \pm i\sqrt{\Delta}. \quad (2.7)$$

Substituting (2.6) into (2.1) and carrying out the integration, we obtain

$$\begin{aligned} \langle x^2 \rangle &= \langle y^2 \rangle = \frac{\hbar}{2\pi m} \operatorname{Im} \left[\frac{1}{\sqrt{\Delta}} \ln \left(\frac{\omega_1}{\omega_2} \right) \right] \\ &= \frac{\hbar}{2\pi m b} \left[2\sqrt{\frac{b+a}{2}} \tan^{-1} \left(\frac{2}{\gamma} \sqrt{\frac{b+a}{2}} \right) + \sqrt{\frac{b-a}{2}} \ln \left(\frac{\gamma/2 + \sqrt{(b-a)/2}}{\gamma/2 - \sqrt{(b-a)/2}} \right) \right], \end{aligned} \quad (2.8)$$

where

$$a = \left(\frac{\omega_c}{2} \right)^2 + \omega_0^2 - \left(\frac{\gamma}{2} \right)^2 \quad \text{and} \quad b = \left[a^2 + \left(\frac{\gamma\omega_c}{2} \right)^2 \right]^{\frac{1}{2}}. \quad (2.9)$$

Setting $\omega_c = 0$ in (2.8), we have

$$\langle z^2 \rangle = \frac{\hbar}{\pi m \sqrt{\omega_0^2 - \gamma^2/4}} \tan^{-1} \left(\frac{2}{\gamma} \sqrt{\omega_0^2 - \gamma^2/4} \right) \quad \text{if } \omega_0 > \frac{\gamma}{2} \quad (2.10)$$

or

$$\langle z^2 \rangle = \frac{\hbar}{2\pi m \sqrt{\gamma^2/4 - \omega_0^2}} \ln \left(\frac{\gamma/2 + \sqrt{\gamma^2/4 - \omega_0^2}}{\gamma/2 - \sqrt{\gamma^2/4 - \omega_0^2}} \right) \quad \text{if } \omega_0 < \frac{\gamma}{2}, \quad (2.11)$$

in agreement with known one-dimensional results in the absence of a magnetic field [77,125].

In order to examine the effect of dissipation on localization, we evaluate the partial derivative of $\langle x^2 \rangle$ with respect to the friction constant γ . From (2.8), it is straightforward to check that

$$\begin{aligned} \frac{\partial}{\partial \gamma} \langle x^2 \rangle = & \frac{\hbar \omega_c}{4\pi m b^2} \left[\frac{b(\gamma^2/4 + (b+a)/2) - (b+a)(\omega_c^2/4 + \omega_0^2 + \gamma^2/4)}{b\sqrt{(b+a)/2}} \tan^{-1} \left(\frac{2}{\gamma} \sqrt{\frac{b+a}{2}} \right) \right. \\ & \left. + \frac{b(\gamma^2/4 - (b-a)/2) - (b-a)(\omega_c^2/4 + \omega_0^2 + \gamma^2/4)}{2b\sqrt{(b-a)/2}} \ln \left(\frac{\gamma/2 + \sqrt{(b-a)/2}}{\gamma/2 - \sqrt{(b-a)/2}} \right) + \gamma \right]. \end{aligned} \quad (2.12)$$

This form is somewhat complicated for the purpose of ascertaining whether it is negative definite or not. Thus we first consider its value at zero dissipation by setting γ to zero in (2.12):

$$\left. \frac{\partial}{\partial \gamma} \langle x^2 \rangle \right|_{\gamma=0} = \frac{\hbar}{2\pi m (\omega_c^2/4 + \omega_0^2)} \left[\frac{\omega_c}{4\sqrt{\omega_c^2/4 + \omega_0^2}} \ln \left(\frac{\sqrt{\omega_c^2/4 + \omega_0^2} + \omega_c/2}{\sqrt{\omega_c^2/4 + \omega_0^2} - \omega_c/2} \right) - 1 \right], \quad (2.13)$$

which can be easily shown to be negative (with a smaller absolute value than the case with $\omega_c = 0$) if $\omega_c < 3.018\omega_0$, but positive if $\omega_c > 3.018\omega_0$. Therefore, for magnetic fields less than the critical value $B_c = mc\omega_c/e = 3.018mc\omega_0/e$, the Ohmic dissipation still results in enhanced localization, but to a less extent than the case without a magnetic field. On the other hand, for a magnetic field surpassing that critical value, the dissipation instead reduces the localization of the oscillator. This result is quite intriguing. It might be understood qualitatively by noting that both the Lorentz force and the frictional force depend on the velocity of the particle, with the latter tending to slow down and hence localize the particle whereas the former tending to delocalize it [see Eq. (2.13)]. It is these opposite tendencies of the dissipation and the magnetic field that give rise to this interesting phenomenon.

In general, the critical value of ω_c is a function of γ for nonzero friction constant, viz., $\omega_c = f(\gamma)$, which is the solution to the equation obtained by setting the right-hand side of (2.12) to zero. From the discussion following (2.13), we immediately have

$f(0) = 3.018\omega_0$. Some other properties of this function can be obtained by analyzing (2.12) in detail.

For both large ω_c and γ (i.e., $\omega_c \gg \omega_0$ and $\gamma \gg \omega_0$), we have, from (2.12),

$$\frac{\partial}{\partial \gamma} \langle x^2 \rangle = \frac{2\hbar}{\pi m} \left[\frac{\omega_c^2 - \gamma^2}{(\omega_c^2 + \gamma^2)^2} \ln \left(\frac{\sqrt{\omega_c^2 + \gamma^2}}{\omega_0} \right) - \frac{\omega_c^2 - \gamma^2}{(\omega_c^2 + \gamma^2)^2} - \frac{2\gamma\omega_c}{(\omega_c^2 + \gamma^2)^2} \tan^{-1} \left(\frac{\omega_c}{\gamma} \right) \right], \quad (2.14)$$

which implies that the leading term of the asymptotic expansion of $f(\gamma)$ is γ , i.e., $f(\gamma) \approx \gamma + \dots$ for $\gamma \gg \omega_0$. Furthermore, taking the derivative of $f(\gamma)$ with respect to γ on both sides of (2.12), we find

$$f'(0) = -\frac{\partial^2}{\partial \gamma^2} \langle x^2 \rangle \Big|_{\gamma=0} / \frac{\partial^2}{\partial \gamma \partial \omega_c} \langle x^2 \rangle \Big|_{\gamma=0} \cong 1.420. \quad (2.15)$$

Finally, we turn to the case of strong dissipation (i.e., $\gamma \gg \omega_0$ and $\gamma \gg \omega_c$) and obtain

$$\langle x^2 \rangle \sim \frac{2\hbar}{\pi m \gamma} \left[\ln \left(\frac{\gamma}{\omega_0} \right) - \frac{\omega_c^2 - 2\omega_0^2}{\gamma^2} \ln \left(\frac{\gamma}{\omega_0} \right) \dots \right]. \quad (2.16)$$

The second leading term in this asymptotic expansion decreases with increasing ω_c . Hence we can see that strong dissipation leads to strong localization and that the magnetic field only slightly enhances this effect.

III. Conclusions

We have calculated explicitly the equal-time position autocorrelation functions, in the presence of a magnetic field \vec{B} , for a charged quantum harmonic oscillator in the Ohmic heat bath. The motion along \vec{B} is unaffected by it, as expected, but the motion perpendicular to it displays an interesting phenomenon due to interplay between the dissipation and the magnetic field \vec{B} . For weak dissipation, the effect of a magnetic field opposes

that of the dissipation. For a \vec{B} field less than a certain critical value, the dissipation effect still dominates over the magnetic-field effect, resulting in a localization weakened by \vec{B} for motion normal to it. However, for a magnetic field larger than this critical value, weak dissipation is simply overwhelmed by the magnetic field, causing an overall reduction in the transversal localization of the particle. Hence the overall shape of the orbit of the oscillator looks somewhat like an oblate ellipsoid with the magnetic field along its symmetry axis. Only in the strong dissipation regime does the magnetic field reinforce the effect of dissipation, leading to stronger localization in the direction orthogonal to the field, and thus the corresponding orbital shape of the oscillator would look more like a football, a symmetric ellipsoid elongated along the direction of the magnetic field.

5. Green's Function and Position Correlation Function in a Heat Bath and a Magnetic Field*

I. Introduction

The problem of dissipative systems in the presence of an external magnetic field is an important but difficult one in solid state physics. Some of the early research topics include the influence of collisions on the magnetic susceptibility of metals [132,133], quantum transport theory for an electron gas in a magnetic field [134], magnetoresistance on the Fermi surface [135,136], electronic conduction in a strong magnetic field [137,138], nuclear magnetic resonance (NMR) [139], relaxation and resonance of spins in zero or low external magnetic fields [140,141], electron-hole pair production and recombination in semiconductors [142], diffusion of nondegenerate charge carriers in a semiconductor [143], and magnetopolaron (i.e., the Fröhlich polaron in the presence of an external magnetic field) [144]. The techniques employed in these studies are mostly the phase-space Fokker-Planck equation for the Wigner function, with the influence of the ambient medium being treated only phenomenologically [145].

*This section consists of the body text of Ref. 158, by X. L. Li and R. F. O'Connell, with its abstract incorporated in Sec. 1 (Introduction to Chapter III) and its references merged into the overall bibliography.

The proper incorporation of dissipation into macroscopic systems, especially in the quantum domain, is by considering the coupled system of the particle involved and its environment, for which detailed microscopic modeling is necessary. Strong impetus to this field was initiated by the pioneering work of Caldeira and Leggett on dissipative quantum tunneling at zero temperature [77]. Since then, the Caldeira–Leggett (C–L) model has been applied to a variety of physical systems to investigate, among others, the asymptotic low temperature properties, which show anomalous behaviors [53].

Meanwhile, the subject of dissipation in a magnetic field has also gained renewed interest over the last decade mainly due to the discovery of highly nonclassical transport of a degenerate Fermi gas in the presence of strong disorder associated with the quantized Hall effect (QHE) [148] and the temperature-dependent normal-state Hall effect in high-temperature superconductors [149]. To understand corrections to the classical form of magnetic properties in such systems, Hong and Wheatley have presented a magnetotransport theory for a charged particle executing quantum diffusion in a two-dimensional, translationally invariant system subject to an external magnetic field, using a somewhat complicated method of diagonalizing the underlying Hamiltonian of the coupled system *à la* Caldeira–Leggett [151].

In this paper, we shall use the much simpler and more transparent approach of the generalized quantum Langevin equation (GLE) based on the neutral independent-oscillator (IO) model of the heat bath [82], which is equivalent to the translationally invariant version of the C–L model required for a free Brownian particle [111]. The problem of a charged quantum particle moving in a scalar potential $V(\vec{r})$, coupled linearly to a passive heat bath, and in the presence of a static external magnetic field \vec{B} , has recently been formulated based on the IO model [152]. The formulation fully incorporates the effects of Landau orbit quantization and the related Landau level structure, thus rendering it unnecessary to make any semiclassical approximation. The linear coupling between particle

and heat bath adopted in the IO model allows the magnetic field to be taken into account nonperturbatively. The ensuing GLE for an isotropic, spatial (three-dimensional) harmonic potential as well as a uniform magnetic field has been solved exactly by means of the Fourier-transformation method, enabling us to obtain integral expressions for many physical quantities such as susceptibilities, symmetrized position correlation functions, and free energies [155]. Here we shall expand that work and focus on two important quantities frequently employed in the study of condensed matter: the retarded Green's functions and the symmetrized position correlation functions. They play prominent roles in the theoretical interpretation of experiments because of their direct relationship with measurable physical quantities and thus are the subject of much interest [117,164].

The rest of this paper is organized as follows. In Sec. II we first introduce the general formalism and notation used in this paper. In particular, we establish several useful properties about the generalized susceptibility tensor $\alpha_{\rho\sigma}(\omega)$ obtained from the GLE for an isotropic harmonic oscillator. We then define the retarded Green's functions as the Fourier transform of the generalized susceptibility tensor and relate them to the nonequal time commutators of position operators. In Sec. III we express, using the fluctuation–dissipation (FD) theorem, the symmetrized position correlation functions in terms of the generalized susceptibility tensor and prove, based on the properties of $\alpha_{\rho\sigma}(\omega)$ just outlined in Sec. II, two general theorems concerning the position autocorrelation functions (dispersions) of motions perpendicular to the external magnetic field that are true for any physical heat baths. In Sec. IV we calculate explicitly the retarded Green's functions and the symmetrized position correlation functions for a harmonic oscillator in the Ohmic heat bath in both classical and quantum limits.

In Sec. V we extend the investigation to the Brownian motion of a charged particle in an external magnetic field. To extract finite results, we introduce the displacement correlation functions, which are related to the symmetrized position correlation functions

but are more appropriate for studying the Brownian motion. We next give a formula for the self-diffusion constant and derive, in the limit of long times at both absolute zero (the quantum regime) and nonzero temperatures (the classical regime), two general relations between the retarded Green's functions and the displacement correlation functions. The classical version of them is a generalization of the Einstein relation and can thus be cast into the form of the Green–Kubo formulas connecting transport coefficients with integrals of appropriate correlation functions. The formulas so developed are subsequently applied to analyze the long-time asymptotic expansion of the displacement correlation functions from that of the retarded Green's functions, for the Ohmic heat bath and a rather general class of frequency-dependent heat baths corresponding to many realistic microscopic models and having therefore been studied extensively, particularly in the context of dissipative quantum phase coherence [99]. Finally, in Sec. VI we summarize our results, compare them with those without a magnetic field, and present our conclusions.

II. Generalized Susceptibility

The quantum Langevin equation for a particle of mass m and charge e in a potential $V(\vec{r})$, and subject to a static external magnetic field \vec{B} takes the form [152]

$$m\ddot{\vec{r}} + \int_{-\infty}^t dt' \mu(t-t') \dot{\vec{r}}(t') + \vec{\nabla} V(\vec{r}) - \frac{e}{c} (\dot{\vec{r}} \times \vec{B}) = \vec{F}(t), \quad (2.1)$$

where the dot denotes differentiation with respect to t . The influence of the external magnetic field \vec{B} is solely represented by the quantum version of the Lorentz-force term, with both the Gaussian random operator-force $\vec{F}(t)$ and the memory function $\mu(t)$ of the heat bath unchanged by the magnetic field.

For a spatial harmonic potential $V(\vec{r}) = (1/2)K\vec{r}^2$ and a uniform magnetic field \vec{B} , the resulting linear operator equation can be exactly solved by the Fourier-transformation method [155]:

$$\tilde{r}_\rho(\omega) = \alpha_{\rho\sigma}(\omega) \tilde{F}_\sigma(\omega) , \quad (2.2)$$

where

$$\begin{aligned} \alpha_{\rho\sigma}(\omega) &\equiv [D(\omega)^{-1}]_{\rho\sigma} \\ &= \left[\lambda^2 \delta_{\rho\sigma} - \left(\omega \frac{e}{c} \right)^2 B_\rho B_\sigma - \epsilon_{\rho\sigma\eta} B_\eta \lambda i \omega \frac{e}{c} \right] / \det D(\omega) \end{aligned} \quad (2.3)$$

with

$$\det D(\omega) = \lambda \left[\lambda^2 - \left(\omega \frac{e}{c} \right)^2 \bar{B}^2 \right] \quad (2.4)$$

and

$$\lambda(\omega) = -m\omega^2 + K - i\omega \tilde{\mu}(\omega) , \quad (2.5)$$

and where $\delta_{\rho\sigma}$ is the Kronecker delta function and $\epsilon_{\rho\sigma\eta}$ is the Levi-Civita symbol. Here we have used tensor notation and shall adopt the Einstein summation convention for repeated indices throughout this paper unless otherwise indicated. The Fourier transform is denoted by a tilde, e.g.,

$$\tilde{\mu}(\omega) \equiv \int_0^\infty dt e^{i\omega t} \mu(t) , \quad (2.6)$$

where, by convention, the memory function $\mu(t)$ vanishes for negative times.

The c-number generalized susceptibility tensor $\alpha_{\rho\sigma}(\omega)$ uniquely determines the dynamics of linear systems. It has the following two useful identities (see Appendix A):

$$\alpha_{\nu\mu}(\omega) - \alpha_{\mu\nu}^*(\omega) = 2i\alpha_{\sigma\mu}(\omega)\alpha_{\sigma\nu}^*(\omega)\omega \operatorname{Re} \tilde{\mu}(\omega) \quad (2.7)$$

and

$$\alpha_{\nu\mu}(\omega) - \alpha_{\mu\nu}^*(\omega) = 2i\alpha_{\nu\sigma}(\omega)\alpha_{\mu\sigma}^*(\omega)\omega \operatorname{Re} \tilde{\mu}(\omega) . \quad (2.8)$$

As with the Fourier transform of the memory function $\tilde{\mu}(\omega)$ [82], $\alpha_{\rho\sigma}(\omega)$ obeys several important properties required by general physical principles. First of all, $\alpha_{\rho\sigma}(\omega)$ satisfies the reality condition [155]

$$\alpha_{\rho\sigma}^*(\omega) = \alpha_{\rho\sigma}(-\omega) , \quad (2.9)$$

which reflects the fact that \tilde{r} is a Hermitian operator. Thus the real and imaginary parts of $\alpha_{\rho\sigma}(\omega)$ are even and odd functions of ω , respectively. Secondly, no element of the matrix $\alpha_{\rho\sigma}(\omega)$ has poles in the upper half-plane (UHP) (see Appendix B). Furthermore, for the three diagonal elements $\alpha_{\rho\rho}(\omega)$ (with $\rho = 1, 2, 3$) we have

$$\text{Im } \alpha_{\rho\rho}(\omega) > 0 \quad \text{for } \omega > 0 , \quad (2.10)$$

thereby $-i\omega\alpha_{\rho\rho}(\omega)$ ($\rho = 1, 2, 3$) are real positive functions (see Appendix C).

The Fourier transform of $\alpha_{\rho\sigma}(\omega)$ is related to the retarded Green's function $G_{\rho\sigma}(t)$:

$$G_{\rho\sigma}(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \alpha_{\rho\sigma}(\omega) . \quad (2.11)$$

The causal Green's functions defined above are very useful for making calculations based on the equations of motion for the operators of interest [165]. They are to be distinguished from another type of Green's function commonly used in statistical physics called a time-ordered Green's function, suitable for the development of diagrammatic perturbation expansions [164].

Inverting the Fourier transform in (2.2) with the aid of (2.11) gives

$$r_{\rho}(t) = \int_{-\infty}^t dt' G_{\rho\sigma}(t-t') [f_{\sigma}(t') + F_{\sigma}(t')] . \quad (2.12)$$

Since $\alpha_{\rho\sigma}(\omega)$ is analytic in the UHP, we see readily from (2.11) that

$$G_{\rho\sigma}(t) = 0 \quad \text{for } t \leq 0. \quad (2.13)$$

This causality property for the retarded Green's function ensures that a response of the system depends only upon the past perturbation.

The retarded Green's function is closely connected with the commutator of position operators. To this end, we need the formula for the commutator between the operator random forces [152]:

$$[F_\rho(t), F_\sigma(t')] = \delta_{\rho\sigma} \frac{2}{i\pi} \int_0^\infty d\omega \operatorname{Re}[\tilde{\mu}(\omega + i0^+)] \hbar \omega \sin[\omega(t - t')]. \quad (2.14)$$

Thereupon we derive the nonequal time commutator of $r_\rho(t)$ and $r_\sigma(t')$ from (2.12)

$$\begin{aligned} [r_\rho(t), r_\sigma(t')] &= \frac{1}{\pi} \int_{-\infty}^\infty d\omega \alpha_{\rho\eta}(\omega) \alpha_{\sigma\eta}^*(\omega) \operatorname{Re}[\tilde{\mu}(\omega)] \hbar \omega e^{-i\omega(t-t')} \\ &= \frac{\hbar}{2\pi i} \int_{-\infty}^\infty d\omega e^{-i\omega(t-t')} [\alpha_{\rho\sigma}(\omega) - \alpha_{\sigma\rho}^*(\omega)], \end{aligned} \quad (2.15)$$

where we have used the inverse Fourier transform of (2.11), and the second equality follows from (2.8).

Applying (2.9) and (2.11) in (2.15) results in

$$[r_\rho(t), r_\sigma(t')] = \frac{\hbar}{i} [G_{\rho\sigma}(t - t') - G_{\sigma\rho}(t' - t)], \quad (2.16)$$

which may also be written, by (2.12), as

$$G_{\rho\sigma}(t) = \frac{i}{\hbar} \theta(t) [r_\rho(t), r_\sigma(0)], \quad (2.17)$$

where $\theta(t)$ is the Heaviside unit step function. Equations (2.16) and (2.17) are familiar in connection with the linear response theory and the fluctuation-dissipation theorem [39]. Note the commutators appearing here are all c-numbers, which is a consequence of

the linearity of the system involved. In accordance, the Green's functions involved are independent of the temperature.

III. Position Correlation Function

The symmetrized position correlation functions may be obtained via the fluctuation-dissipation theorem [43,88]

$$\begin{aligned}
 \psi_{\rho\sigma}(t-t') &\equiv \frac{1}{2} \langle r_{\rho}(t)r_{\sigma}(t') + r_{\sigma}(t')r_{\rho}(t) \rangle \\
 &= \frac{\hbar}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{1}{2i} [\alpha_{\rho\sigma}(\omega + i0^+) - \alpha_{\sigma\rho}^*(\omega + i0^+)] \coth\left(\frac{\hbar\omega}{2kT}\right) e^{-i\omega(t-t')} \\
 &= \frac{\hbar}{\pi} \int_0^{\infty} d\omega \operatorname{Im}[\alpha_{\rho\sigma}^s(\omega + i0^+)] \coth\left(\frac{\hbar\omega}{2kT}\right) \cos[\omega(t-t')] \\
 &\quad - \frac{\hbar}{\pi} \int_0^{\infty} d\omega \operatorname{Re}[\alpha_{\rho\sigma}^a(\omega + i0^+)] \coth\left(\frac{\hbar\omega}{2kT}\right) \sin[\omega(t-t')], \tag{3.1}
 \end{aligned}$$

where

$$\alpha_{\rho\sigma}^s(\omega) \equiv \frac{1}{2} [\alpha_{\rho\sigma}(\omega) + \alpha_{\sigma\rho}(\omega)] = \left[\lambda^2 \delta_{\rho\sigma} - \left(\omega \frac{e}{c} \right)^2 B_{\rho} B_{\sigma} \right] / \det D(\omega) \tag{3.2}$$

and

$$\alpha_{\rho\sigma}^a(\omega) \equiv \frac{1}{2} [\alpha_{\rho\sigma}(\omega) - \alpha_{\sigma\rho}(\omega)] = \left(-\epsilon_{\rho\sigma\eta} B_{\eta} \lambda i \omega \frac{e}{c} \right) / \det D(\omega) \tag{3.3}$$

are the symmetric and antisymmetric parts of $\alpha_{\rho\sigma}(\omega)$, respectively; k in front of temperature T denotes the Boltzmann constant; and the last equality in (3.1) is obtained with use of the reality condition (2.9) on $\alpha_{\rho\sigma}^s(\omega)$ and $\alpha_{\rho\sigma}^a(\omega)$. We note here that $\alpha_{\rho\sigma}^s(\omega)$ and $\alpha_{\rho\sigma}^a(\omega)$ as defined in (3.2) and (3.3), respectively, possess the same properties as those for $\alpha_{\rho\sigma}(\omega)$, namely, (2.9), (2.10), and (2.11), which can easily be verified. For definiteness, we shall choose the direction of the magnetic field as z direction in calculations throughout this paper. Then, from (2.3), the only nonzero elements of $\alpha_{\rho\sigma}(\omega)$ are

α_{11} , α_{22} , α_{33} , α_{12} , and α_{21} , which, due to the cylindrical symmetry of the system, are related to each other by

$$\alpha_{11}(\omega) = \alpha_{22}(\omega) = \lambda^2 / \det D(\omega) \quad (3.4)$$

and

$$\alpha_{12}(\omega) = -\alpha_{21}(\omega) = -i\omega \frac{e}{c} B \lambda / \det D(\omega). \quad (3.5)$$

There follows from (2.11), (3.1), (3.4), and (3.5) that the cross retarded Green's function $G_{12}(t)$ and the position cross-correlation function $\psi_{12}(t)$ are both identically zero if no magnetic field is present, as expected.

The position autocorrelation functions (also called dispersions) of the motions both perpendicular and parallel to the magnetic field \vec{B} are given by the equal-time values of the diagonal elements of $\psi_{\rho\sigma}(t)$ in (3.1)

$$\langle x^2 \rangle = \langle y^2 \rangle = \frac{\hbar}{\pi} \int_0^\infty d\omega \operatorname{Im} \alpha_{11}(\omega) \coth\left(\frac{\hbar\omega}{2kT}\right) \quad (3.6)$$

and

$$\langle z^2 \rangle = \frac{\hbar}{\pi} \int_0^\infty d\omega \operatorname{Im} \alpha_{33}(\omega) \coth\left(\frac{\hbar\omega}{2kT}\right), \quad (3.7)$$

and it is easy to verify that $\langle z^2 \rangle$ may simply be obtained by setting \vec{B} to zero in (3.6) for $\langle x^2 \rangle$ or $\langle y^2 \rangle$, which is a consequence of the fact that a magnetic field does not affect motions parallel to it.

The factor $\coth(\hbar\omega/2kT)$ in (3.6) is a monotonically increasing function of temperature T , so are $\langle x^2 \rangle$ and $\langle y^2 \rangle$ as deduced from (3.6) and (2.10), i.e.,

$$\frac{\partial}{\partial T} \langle x^2 \rangle = \frac{\partial}{\partial T} \langle y^2 \rangle > 0. \quad (3.8)$$

The same holds for $\langle z^2 \rangle$ as in the one-dimensional case [125].

The dispersions $\langle x^2 \rangle$ or $\langle y^2 \rangle$ may also be expressed in a series form by means of the theorem of residues from the theory of functions of a complex variable. First, noting that the integrand in (3.6) is an even function of ω because of the reality condition (2.9) on $\alpha_{11}(\omega)$, (3.6) can be rewritten as

$$\langle x^2 \rangle = \frac{\hbar}{2\pi i} \int_{-\infty}^{\infty} d\omega \alpha_{11}(\omega) \coth\left(\frac{\hbar\omega}{2kT}\right). \quad (3.9)$$

We may now close the contour in the UHP, where only the factor $\coth(\hbar\omega/2kT)$ in the integrand in (3.9) contributes simple poles at $\omega = i\nu_n$ ($n=1,2,\dots$). Here $\nu_n = (2\pi kT/\hbar)n$ are the usual Matsubara frequencies [129]. The summation over the residues yields

$$\langle x^2 \rangle = \frac{kT}{m} \left[\frac{1}{\omega_0^2} + 2 \sum_{n=1}^{\infty} \frac{\hat{\lambda}(\nu_n)}{\hat{\lambda}^2(\nu_n) + (\nu_n \omega_c)^2} \right], \quad (3.10)$$

where $\omega_c \equiv eB/mc$ is the cyclotron frequency and $\omega_0^2 = (K/m)^{1/2}$ is the bare-oscillator frequency, and where

$$\hat{\lambda}(\nu_n) \equiv \lambda(i\nu_n)/m = \nu_n^2 + \omega_0^2 + \nu_n \hat{\gamma}(\nu_n) \quad (3.11)$$

with

$$\hat{\gamma}(\nu_n) \equiv \tilde{\mu}(i\nu_n)/m. \quad (3.12)$$

Since $\tilde{\mu}(iz) > 0$ for $z > 0$ [82], it follows from (3.11) and (3.12) that $\hat{\lambda}(\nu_n) > 0$ ($n=1,2,\dots$). Therefore $\langle x^2 \rangle$ decreases monotonically with increasing strength of the magnetic field

$$\frac{\partial}{\partial B} \langle x^2 \rangle < 0. \quad (3.13)$$

We conclude this section by emphasizing that the Eqs. (3.8) and (3.13) hold for any strength of a magnetic field and any type of heat baths restricted only by general

physical principles. Equation (3.13) is also closely related to the fact that the dissipative system of a charged quantum oscillator in an external magnetic field is still generally diamagnetic (see Appendix D).

IV. Charged Oscillator in an Ohmic Heat Bath and a Magnetic Field

For a strict Ohmic heat bath, the memory function $\tilde{\mu}(\omega) = m\gamma$ is frequency independent. Bearing in mind that $\tilde{\mu}(\omega)$ is a property of heat bath only, the friction coefficient γ thus defined is actually inversely proportional to the particle's mass m . The retarded Green's functions defined in (2.11), with the aid of (2.3)–(2.5), may now be evaluated by the method of contour integration:

$$\begin{aligned} G_{11}(t) &= -\frac{1}{4\pi m} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \left[\frac{1}{\omega^2 - \omega_0^2 + i\gamma\omega + \omega_c\omega} + \frac{1}{\omega^2 - \omega_0^2 + i\gamma\omega - \omega_c\omega} \right] \\ &= \frac{1}{2mb} \theta(t) \left\{ \exp(-\Omega_4 t) \left[\sqrt{\frac{b+a}{2}} \sin(\Omega_2 t) + \sqrt{\frac{b-a}{2}} \cos(\Omega_2 t) \right] \right. \\ &\quad \left. + \exp(-\Omega_3 t) \left[\sqrt{\frac{b+a}{2}} \sin(\Omega_1 t) - \sqrt{\frac{b-a}{2}} \cos(\Omega_1 t) \right] \right\} \end{aligned} \quad (4.1)$$

and

$$\begin{aligned} G_{12}(t) &= -\frac{1}{4\pi im} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \left[\frac{1}{\omega^2 - \omega_0^2 + i\gamma\omega + \omega_c\omega} - \frac{1}{\omega^2 - \omega_0^2 + i\gamma\omega - \omega_c\omega} \right] \\ &= \frac{1}{2mb} \theta(t) \left\{ \exp(-\Omega_4 t) \left[\sqrt{\frac{b+a}{2}} \cos(\Omega_2 t) - \sqrt{\frac{b-a}{2}} \sin(\Omega_2 t) \right] \right. \\ &\quad \left. - \exp(-\Omega_3 t) \left[\sqrt{\frac{b+a}{2}} \cos(\Omega_1 t) + \sqrt{\frac{b-a}{2}} \sin(\Omega_1 t) \right] \right\}, \end{aligned} \quad (4.2)$$

where

$$\Omega_{1,2} = \sqrt{\frac{b+a}{2}} \pm \frac{\omega_c}{2} \quad \text{and} \quad \Omega_{3,4} = \frac{\gamma}{2} \pm \sqrt{\frac{b-a}{2}} \quad (4.3)$$

are four nonnegative frequencies, and where

$$a = \left(\frac{\omega_c}{2}\right)^2 + \omega_0^2 - \left(\frac{\gamma}{2}\right)^2 \quad (4.4)$$

and

$$b = \left[a^2 + \left(\frac{\gamma\omega_c}{2}\right)^2 \right]^{\frac{1}{2}}. \quad (4.5)$$

Setting $\omega_c = 0$, we arrive at the familiar result for a one-dimensional damped harmonic oscillator in the absence of an external magnetic field

$$G_{33}(t) = \begin{cases} \frac{1}{m\sqrt{\omega_0^2 - \gamma^2/4}} \theta(t) \exp\left(-\frac{\gamma}{2}t\right) \sin\left(t\sqrt{\omega_0^2 - \gamma^2/4}\right) & \text{if } \omega_0 > \frac{\gamma}{2} \\ \frac{1}{m\sqrt{\gamma^2/4 - \omega_0^2}} \theta(t) \exp\left(-\frac{\gamma}{2}t\right) \sin\left(t\sqrt{\gamma^2/4 - \omega_0^2}\right) & \text{if } \omega_0 < \frac{\gamma}{2}. \end{cases} \quad (4.6)$$

Next we calculate the symmetrized position correlation functions $\psi_{\rho\sigma}(t)$ in (3.1)

by the method of contour integration. The results are

$$\begin{aligned} \psi_{11}(t) = & -\frac{\hbar}{4m} \text{Im} \left\{ \frac{1}{\zeta} \left[\cot\left(\frac{\hbar\omega_1}{2kT}\right) e^{-\omega_1\tau} - \cot\left(\frac{\hbar\omega_2}{2kT}\right) e^{-\omega_2\tau} \right] \right\} \\ & -\frac{\hbar}{4\pi m} \text{Im} \left\{ \frac{1}{\zeta} \left[\frac{1}{\bar{\omega}_1} F(1, \bar{\omega}_1; 1 + \bar{\omega}_1; e^{-\nu_1\tau}) - \frac{1}{\bar{\omega}_1} F(1, -\bar{\omega}_1; 1 - \bar{\omega}_1; e^{-\nu_1\tau}) \right. \right. \\ & \left. \left. - \frac{1}{\bar{\omega}_2} F(1, \bar{\omega}_2; 1 + \bar{\omega}_2; e^{-\nu_2\tau}) + \frac{1}{\bar{\omega}_2} F(1, -\bar{\omega}_2; 1 - \bar{\omega}_2; e^{-\nu_2\tau}) \right] \right\} \end{aligned} \quad (4.7)$$

and

$$\begin{aligned} \psi_{12}(t) = & \frac{\hbar}{4m} \text{sign}(t) \text{Re} \left\{ \frac{1}{\zeta} \left[\cot\left(\frac{\hbar\omega_1}{2kT}\right) e^{-\omega_1\tau} - \cot\left(\frac{\hbar\omega_2}{2kT}\right) e^{-\omega_2\tau} \right] \right\} \\ & -\frac{\hbar}{4\pi m} \text{sign}(t) \text{Re} \left\{ \frac{1}{\zeta} \left[\frac{1}{\bar{\omega}_1} F(1, \bar{\omega}_1; 1 + \bar{\omega}_1; e^{-\nu_1\tau}) + \frac{1}{\bar{\omega}_1} F(1, -\bar{\omega}_1; 1 - \bar{\omega}_1; e^{-\nu_1\tau}) \right. \right. \\ & \left. \left. - \frac{1}{\bar{\omega}_2} F(1, \bar{\omega}_2; 1 + \bar{\omega}_2; e^{-\nu_2\tau}) - \frac{1}{\bar{\omega}_2} F(1, -\bar{\omega}_2; 1 - \bar{\omega}_2; e^{-\nu_2\tau}) \right] \right\}, \end{aligned} \quad (4.8)$$

where

$$\omega_{1,2} = \frac{\gamma - i\omega_c}{2} \pm i\zeta \quad (4.9)$$

and

$$\zeta = \sqrt{\frac{b+a}{2}} + i\sqrt{\frac{b-a}{2}}, \quad (4.10)$$

and where $\bar{\omega}_{1,2} \equiv \hbar\omega_{1,2}/2\pi kT$ are the corresponding temperature-reduced dimensionless frequencies; $\nu_1 = 2\pi kT/\hbar$; τ is the absolute value of t , $\tau = |t|$; $\text{sign}(t)$ is the sign function, $\text{sign}(t) = t/|t|$; and $F(a, b; c; z)$ is the Gauss hypergeometric function [130].

To simplify the above formulas, we now discuss the high-temperature limit $kT \gg \hbar\omega_{1,2}$, where the first two terms in (4.7) and (4.8) dominate. Comparing (4.3) with (4.9) and (4.10), we see that $\omega_{1,2}$ is connected with $\Omega_{1,2,3,4}$ by

$$\omega_1 = \Omega_4 + i\Omega_2 \quad \text{and} \quad \omega_2 = \Omega_3 - i\Omega_1. \quad (4.11)$$

From (4.7), (4.8), and (4.11), we get the classical results

$$\begin{aligned} \psi_{11}(t) = \frac{kT}{2m\omega_0^2 b} \{ & [(b-f)\cos(\Omega_1\tau) + g\sin(\Omega_1\tau)]e^{-\Omega_1\tau} \\ & + [(b+f)\cos(\Omega_2\tau) + g\sin(\Omega_2\tau)]e^{-\Omega_2\tau} \} \end{aligned} \quad (4.12)$$

and

$$\begin{aligned} \psi_{12}(t) = \frac{kT}{2m\omega_0^2 b} \text{sign}(t) \{ & [(b-f)\sin(\Omega_1\tau) - g\cos(\Omega_1\tau)]e^{-\Omega_1\tau} \\ & - [(b+f)\sin(\Omega_2\tau) - g\cos(\Omega_2\tau)]e^{-\Omega_2\tau} \}, \end{aligned} \quad (4.13)$$

where

$$f \equiv \frac{\omega_c}{2} \sqrt{\frac{b+a}{2}} + \frac{\gamma}{2} \sqrt{\frac{b-a}{2}} \quad \text{and} \quad g \equiv \frac{\gamma}{2} \sqrt{\frac{b+a}{2}} - \frac{\omega_c}{2} \sqrt{\frac{b-a}{2}}.$$

In the low-temperature regime $kT \ll \hbar\omega_{1,2}$, on the other hand, the hypergeometric functions in (4.7) and (4.8) become important. At $T = 0$ K, the summations in the serial expansion of the hypergeometric functions are replaced by continuous integrals and, from (3.1), we find for $\psi_{\rho\sigma}(t)$

$$\psi_{11}(t) = \frac{1}{4\pi m} \text{Im} \left\{ \frac{1}{\zeta} \left[e^{\omega_1 \tau} E_1(\omega_2 \tau) + e^{-\omega_2 \tau} E_1(-\omega_2 \tau) - e^{\omega_1 \tau} E_1(\omega_1 \tau) - e^{-\omega_1 \tau} E_1(-\omega_1 \tau) + i\pi(e^{-\omega_1 \tau} + e^{-\omega_2 \tau}) \right] \right\} \quad (4.14)$$

and

$$\psi_{12}(t) = -\frac{\hbar}{4\pi m} \text{Re} \left\{ \frac{1}{\zeta} \left[e^{\omega_1 t} E_1(\omega_1 t) - e^{-\omega_1 t} E_1(-\omega_1 t) - e^{\omega_2 t} E_1(\omega_2 t) + e^{-\omega_2 t} E_1(-\omega_2 t) + i\pi \text{sign}(t)(e^{-\omega_1 \tau} + e^{-\omega_2 \tau}) \right] \right\}, \quad (4.15)$$

where $E_1(z) \equiv \int_z^\infty dt t^{-1} e^{-t}$ ($|\arg z| < \pi$) is the exponential integral function, which is single-valued with the cut line along the negative axis [130]. For $t \gg 1/\gamma$, we recover the power law for the long-time tail characteristic of Ohmic dissipation [166]:

$$\psi_{11}(t) = -\frac{\hbar\gamma}{\pi m \omega_0^4 t^2} + O(t^{-4}) \quad (4.16)$$

and

$$\psi_{12}(t) = \frac{4\hbar\gamma\omega_c}{\pi m \omega_0^6 t^3} + O(t^{-5}). \quad (4.17)$$

We note here that the leading-order t^{-2} term in (4.16) for the symmetrized position auto-correlation functions in the plane perpendicular to \vec{B} at zero temperature is unchanged by the magnetic field.

We end this section by considering the dispersion of the position operator $\langle x^2 \rangle$, which could be obtained by putting $t = 0$ in (4.7)

$$\langle x^2 \rangle = \frac{kT}{m\omega_0^2} + \frac{1}{2\pi m} \text{Im} \left\{ \frac{1}{\zeta} [\psi(1 + \bar{\omega}_1) - \psi(1 + \bar{\omega}_2)] \right\}, \quad (4.18)$$

where $\psi(z)$ is the logarithmic derivative of the gamma function $\Gamma(z)$ [130]. The equal-time value of the position cross-correlation function $\psi_{12}(t)$, in comparison, is zero as seen from (3.1) and (3.6). In the high-temperature region $kT \gg \hbar\omega_{1,2}$, by expanding the $\psi(z)$ functions involved about 1, (4.18) reduces to

$$\langle x^2 \rangle = \frac{kT}{m\omega_0^2} + O(T^{-1}), \quad (4.19)$$

in accord with the classical equipartition law since the phenomenon of magnetism is quantum-mechanical in nature. While for low temperatures $kT \ll \hbar\omega_{1,2}$, we may insert the asymptotic expansion of $\psi(z)$ in (4.18) and find

$$\begin{aligned} \langle x^2 \rangle = \frac{\hbar}{2\pi mb} & \left\{ 2\sqrt{\frac{b+a}{2}} \tan^{-1} \left(\frac{2}{\gamma} \sqrt{\frac{b+a}{2}} \right) + \sqrt{\frac{b-a}{2}} \ln \left[\frac{\gamma/2 + \sqrt{(b-a)/2}}{\gamma/2 - \sqrt{(b-a)/2}} \right] \right\} \\ & + \frac{\pi\gamma(kT)^2}{3\hbar m\omega_0^4} + O(kT)^4, \end{aligned} \quad (4.20)$$

which has the T^2 power-law correction characteristic of the Ohmic heat bath. We note in passing that this leading-order correction term is independent of the magnetic field.

V. Quantum Brownian Motion of a Charged Particle in a Magnetic Field

A. Relations between $d_{\rho\sigma}(t)$ and $G_{\rho\sigma}(t)$ at long times

The Brownian motion is a special case of damped harmonic oscillator considered previously. As we take the limit $\omega_0 = 0$ in (3.1), the symmetrized position correlation functions $\psi_{\rho\sigma}(t)$ become infrared-divergent, reflecting the fact that the coordinates of a free particle are unbounded. To extract finite results, we introduce the displacement correlation functions according to

$$d_{\rho\sigma}(t) = 2[\psi_{\rho\sigma}(0) - \psi_{\rho\sigma}(t)], \quad (5.1)$$

which is physically more meaningful here. Its diagonal elements, from (3.1), are the mean square displacements in each direction

$$d_{\rho\rho}(t) = \langle (r_\rho(t) - r_\rho(0))^2 \rangle \quad \text{for } \rho = 1, 2, 3. \quad (5.2)$$

Taking the time derivatives in (3.1) and (5.1), we then have

$$\begin{aligned} \dot{d}_{\rho\sigma}(t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \hbar \omega \coth\left(\frac{\hbar\omega}{2kT}\right) [\alpha_{\rho\sigma}(\omega + i0^+) - \alpha_{\sigma\rho}^*(\omega + i0^+)] e^{-i\omega t} \\ &= \frac{2\hbar}{\pi} \int_0^{\infty} d\omega \omega \coth\left(\frac{\hbar\omega}{2kT}\right) [\text{Im } \alpha_{\rho\sigma}^s(\omega) \sin(\omega t) + \text{Re } \alpha_{\rho\sigma}^a(\omega) \cos(\omega t)]. \end{aligned} \quad (5.3)$$

In the long-time limit $t \rightarrow \infty$, at finite temperature T , the small-frequency contributions dominate in (5.3). By expanding the factor $\coth(\hbar\omega/2kT)$ about $\omega = 0$ and employing the definition (2.11) for the retarded Green's functions, we obtain the following simple relation between $d_{\rho\sigma}(t)$ and $G_{\rho\sigma}(t)$

$$\dot{d}_{\rho\sigma}(t) = 2kTG_{\rho\sigma}(t) \quad \text{for } t \rightarrow \infty \text{ and } T > 0, \quad (5.4)$$

where we have used the fact that $\alpha_{\rho\sigma}(\omega)$ is analytic in the UHP and so is $\alpha_{\sigma\rho}^*(\omega)$ in the lower half-plane (LHP).

The significance of (5.4) may be appreciated by introducing linear dc mobility tensor $(\mu_l)_{\rho\sigma}$ and diffusion-coefficient tensor $D_{\rho\sigma}$ [53]. For a constant external force \bar{f} switched on at $t = 0$, we get from the Fourier transform of (2.2), after adding \bar{f} to its right-hand side and averaging out the random force \bar{F} , $\langle r_\rho(t) \rangle = \left\{ \int_0^t G_{\rho\sigma}(s) ds \right\} f_\sigma$, so that the drift velocity of the particle is directly related to $G_{\rho\sigma}(t)$ by

$$\langle \dot{r}_\rho(t) \rangle = G_{\rho\sigma}(t) f_\sigma \quad \text{for } t > 0. \quad (5.5)$$

The linear dc mobility tensor $(\mu_l)_{\rho\sigma}$ is defined through the asymptotic relation $\lim_{t \rightarrow \infty} \langle \dot{r}_\rho(t) \rangle = (\mu_l)_{\rho\sigma} f_\sigma$, yielding, from (5.5), (2.11), (2.3)–(2.5),

$$\begin{aligned} (\mu_l)_{\rho\sigma} &= \lim_{t \rightarrow \infty} G_{\rho\sigma}(t) = \lim_{\omega \rightarrow 0} (-i\omega) \alpha_{\rho\sigma}(\omega) \\ &= \left[\tilde{\gamma}^2(0) \delta_{\rho\sigma} + \left(\frac{e}{mc} \right)^2 B_\rho B_\sigma + \varepsilon_{\rho\sigma\eta} B_\eta \tilde{\gamma}(0) \frac{e}{mc} \right] / \left\{ m \tilde{\gamma}(0) [\tilde{\gamma}^2(0) + \omega_c^2] \right\}, \end{aligned} \quad (5.6)$$

where $\tilde{\gamma}(0) \equiv \tilde{\mu}(0)/m$ and we have assumed in the last line that $\tilde{\mu}(0) \neq 0$. On the other hand, the diffusion-coefficient tensor $D_{\rho\sigma}$ is defined in the standard way by

$$D_{\rho\sigma} \equiv \frac{1}{2} \lim_{t \rightarrow \infty} \dot{d}_{\rho\sigma}(t). \quad (5.7)$$

With the aid of (5.6) and (5.7), (5.4) may be recast as

$$D_{\rho\sigma} = kT (\mu_l)_{\rho\sigma} \quad \text{for } T \neq 0, \quad (5.8)$$

which is a generalized version of the Einstein relation [9].

The diffusion-coefficient tensor could also be derived in another way. For this purpose, we calculate the velocity correlation functions in the classical regime from the corresponding position correlation functions

$$\langle v_\rho(t) v_\sigma(t') \rangle = \partial_{t'} \partial_t \psi_{\rho\sigma}(t - t'), \quad (5.9)$$

where ∂_t denotes partial derivative with respect to t and where we have already exploited the fact that the commutator of two operators is of the order of \hbar in reducing the symmetrized correlation functions for quantum operators to the simple correlation functions for the same variables in the classical regime.

Substituting (3.1) in (5.9), we find for $kT \gg \hbar/t$

$$\begin{aligned} \langle v_\rho(t) v_\sigma(0) \rangle &= \frac{kT}{2\pi i} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \omega [\alpha_{\rho\sigma}(\omega) - \alpha_{\sigma\rho}^*(\omega)] \\ &= \frac{kT}{2\pi i} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \omega \alpha_{\rho\sigma}(\omega) \\ &= \frac{kT}{\pi i} \int_{-\infty}^{\infty} d\omega \cos(\omega t) \omega \alpha_{\rho\sigma}(\omega) \quad \text{for } t \geq 0, \end{aligned} \quad (5.10)$$

where the last two equalities are obtained by using for positive t the analyticity of $\alpha_{\rho\sigma}(\omega)$ and $\alpha_{\sigma\rho}^*(\omega)$ in the UHP and LHP, respectively.

Integrating both sides of (5.10) from 0 to $+\infty$ and employing the integral representation of the Dirac delta function yields

$$\int_0^\infty dt \langle v_\rho(t) v_\sigma(0) \rangle = -ikT \int_{-\infty}^{\infty} d\omega \omega \alpha_{\rho\sigma}(\omega) \delta(\omega) = kT \lim_{\omega \rightarrow 0} (-i\omega) \alpha_{\rho\sigma}(\omega). \quad (5.11)$$

Comparing (5.11) with (5.6) and (5.8), we obtain

$$D_{\rho\sigma} = \int_0^\infty dt \langle v_\rho(t) v_\sigma(0) \rangle, \quad (5.12)$$

which is just the Green-Kubo-type formula connecting transport coefficients with integrals of appropriate correlation functions [4,28].

The situation at zero temperature, once again, has to be treated separately. From (3.1) and (5.1) one finds for the displacement correlation functions at $T = 0$

$$d_{\rho\sigma}(t) = \frac{2\hbar}{\pi} \int_0^\infty d\omega \left\{ \text{Im } \alpha_{\rho\sigma}^s(\omega) [1 - \cos(\omega t)] + \text{Re } \alpha_{\rho\sigma}^a(\omega) \sin(\omega t) \right\}, \quad (5.13)$$

which, by virtue of the identities [167]

$$\sin(\omega t) = \frac{2}{\pi} \int_0^\infty dy \frac{1}{y^2 - 1} \cos\left(\frac{\omega t}{y}\right)$$

and

$$1 - \cos(\omega t) = \frac{2}{\pi} \int_0^\infty dy \frac{y}{y^2 - 1} \sin\left(\frac{\omega t}{y}\right), \quad (5.14)$$

can be related to $G_{\rho\sigma}(t)$ by

$$d_{\rho\sigma}(t) = \frac{2\hbar}{\pi} \int_0^\infty dy \frac{1}{y^2 - 1} \left[y G_{\rho\sigma}^s\left(\frac{t}{y}\right) + G_{\rho\sigma}^a\left(\frac{t}{y}\right) \right] \quad \text{for } T = 0, \quad (5.15)$$

where $G_{\rho\sigma}^s(t)$ and $G_{\rho\sigma}^a(t)$ are the symmetric and antisymmetric parts of $G_{\rho\sigma}(t)$ corresponding, through (2.11), to $\alpha_{\rho\sigma}^s$ and $\alpha_{\rho\sigma}^a$ defined in (3.2) and (3.3), respectively. If $G_{\rho\sigma}^s(t)$ and $G_{\rho\sigma}^a(t)$ are finite when $t \rightarrow \infty$, i.e., finite mobility (as for the Ohmic heat bath), then, upon splitting the integral in (5.15) into one from 0 to t and a remaining correction term, one obtains to the leading-order term

$$d_{\rho\sigma}(t) = \frac{2\hbar}{\pi} G_{\rho\sigma}^s(+\infty) \ln(t) \quad \text{for } t \rightarrow \infty \text{ and } T = 0. \quad (5.16)$$

The contribution of $G_{\rho\sigma}^a(+\infty)$ to (5.16) is proportional to t^{-1} .

B. Ohmic heat bath

The results for a charged Brownian particle in an Ohmic heat bath and in the presence of an external magnetic field may simply be derived by taking the limit $\omega_0^2 \rightarrow 0$ in the corresponding formulas for a charged oscillator in Sec. IV. From (4.1) and (4.2), the retarded Green's functions read

$$G_{11}(t) = \frac{1}{m(\omega_c^2 + \gamma^2)} \left\{ \gamma + e^{-\gamma t} [\omega_c \sin(\omega_c t) - \gamma \cos(\omega_c t)] \right\} \theta(t) \quad (5.17)$$

and

$$G_{12}(t) = \frac{1}{m(\omega_c^2 + \gamma^2)} \left\{ \omega_c - e^{-\gamma t} [\omega_c \cos(\omega_c t) + \gamma \sin(\omega_c t)] \right\} \theta(t). \quad (5.18)$$

Combining (4.7), (4.8), and (5.1), we find for the displacement correlation functions of a Brownian particle

$$\begin{aligned}
 d_{11}(t) = & \frac{2kT\gamma\tau}{m(\gamma^2 + \omega_c^2)} - \frac{2kT(\gamma^2 - \omega_c^2)}{m(\gamma^2 + \omega_c^2)^2} + \frac{\hbar e^{-\gamma\tau}}{m(\gamma^2 + \omega_c^2)} \left\{ \sin\left(\frac{\hbar\gamma}{kT}\right) [\gamma \cos(\omega_c\tau) - \omega_c \sin(\omega_c\tau)] \right. \\
 & \left. - \sinh\left(\frac{\hbar\omega_c}{kT}\right) [\gamma \sin(\omega_c\tau) + \omega_c \cos(\omega_c\tau)] \right\} / \left[\cosh\left(\frac{\hbar\omega_c}{kT}\right) - \cos\left(\frac{\hbar\gamma}{kT}\right) \right] \\
 & + \frac{4kT}{m} \sum_{n=1}^{\infty} \frac{v_n + \gamma}{v_n[(v_n + \gamma)^2 + \omega_c^2]} + \frac{4kT}{m} \sum_{n=1}^{\infty} \frac{\gamma(v_n^2 - \gamma^2 - \omega_c^2)e^{-v_n\tau}}{v_n[(v_n^2 - \gamma^2 + \omega_c^2)^2 + 4\gamma^2\omega_c^2]}
 \end{aligned} \tag{5.19}$$

and

$$\begin{aligned}
 d_{12}(t) = & \frac{2kT\omega_c t}{m(\gamma^2 + \omega_c^2)} - \text{sign}(t) \frac{4kT\gamma\omega_c}{m(\gamma^2 + \omega_c^2)^2} - \text{sign}(t) \frac{8kT}{m} \sum_{n=1}^{\infty} \frac{\gamma\omega_c e^{-v_n\tau}}{(v_n^2 - \gamma^2 + \omega_c^2)^2 + 4\gamma^2\omega_c^2} \\
 & + \text{sign}(t) \frac{\hbar e^{-\gamma\tau}}{m(\gamma^2 + \omega_c^2)} \left\{ \sin\left(\frac{\hbar\gamma}{kT}\right) [\gamma \sin(\omega_c\tau) + \omega_c \cos(\omega_c\tau)] \right. \\
 & \left. + \sinh\left(\frac{\hbar\omega_c}{kT}\right) [\gamma \cos(\omega_c\tau) - \omega_c \sin(\omega_c\tau)] \right\} / \left[\cosh\left(\frac{\hbar\omega_c}{kT}\right) - \cos\left(\frac{\hbar\gamma}{kT}\right) \right].
 \end{aligned} \tag{5.20}$$

In the classical regime ($kT \gg \hbar\gamma$ and $kT \gg \hbar\omega_c$), these simplify to the expressions

$$\begin{aligned}
 d_{11}(t) = & \frac{2kT}{m(\gamma^2 + \omega_c^2)} \left\{ \gamma\tau - \frac{\gamma^2 - \omega_c^2}{\gamma^2 + \omega_c^2} \right. \\
 & \left. + \frac{e^{-\gamma\tau}}{\gamma^2 + \omega_c^2} [(\gamma^2 - \omega_c^2)\cos(\omega_c\tau) - 2\gamma\omega_c\sin(\omega_c\tau)] \right\}
 \end{aligned} \tag{5.21}$$

and

$$d_{12}(t) = \frac{2kT}{m(\gamma^2 + \omega_c^2)} \left\{ \omega_c t - \text{sign}(t) \frac{2\gamma\omega_c}{\gamma^2 + \omega_c^2} + \text{sign}(t) \frac{e^{-\gamma\tau}}{\gamma^2 + \omega_c^2} \left[(\gamma^2 - \omega_c^2) \sin(\omega_c \tau) + 2\gamma\omega_c \cos(\omega_c \tau) \right] \right\}, \quad (5.22)$$

upon which, by inserting (5.1) into (5.9), we readily arrive at the velocity correlation functions at high temperatures

$$\langle v_1(t)v_1(0) \rangle = \frac{1}{2} \ddot{d}_{11}(t) = \frac{kT}{m} \cos(\omega_c t) \exp(-\gamma\tau) \quad (5.23)$$

and

$$\langle v_1(t)v_2(0) \rangle = \frac{1}{2} \ddot{d}_{12}(t) = \frac{kT}{m} \sin(\omega_c t) \exp(-\gamma\tau). \quad (5.24)$$

The exponential decay for the velocity correlation functions is characteristic of the theory of Langevin equation [16,17], as long as the time t involved is not too small (compared to the mean time between atomic collisions) [168]. Substituting (5.23) and (5.24) in (5.12) gives

$$D_{11} = \frac{kT}{m} \frac{\gamma}{\gamma^2 + \omega_c^2} \quad (5.25)$$

and

$$D_{12} = \frac{kT}{m} \frac{\omega_c}{\gamma^2 + \omega_c^2}, \quad (5.26)$$

which is, of course, in accord with the direct evaluation of (5.6) in (5.8). The magnetic field manifests itself as a multiplicative term oscillating with the cyclotron frequency for the velocity correlation functions of a charged Brownian particle in the plane perpendicular to the field and the self-diffusion constants are reduced by a cofactor dependent on the magnetic field.

In the quantum regime ($t \ll \hbar/kT$, $kT \ll \hbar\gamma$ and $kT \ll \hbar\omega_c$), on the other hand, the series terms in (5.19) and (5.20) are important. From (4.14), (4.15), and (5.1), after taking the $\omega_0^2 \rightarrow 0$ limit, we obtain for a Brownian particle at $T = 0$

$$\begin{aligned}
 d_{11}(t) = & \frac{2\hbar}{\pi m(\gamma^2 + \omega_c^2)} \left[\gamma \ln \left(\tau \sqrt{\gamma^2 + \omega_c^2} \right) + C\gamma + \omega_c \tan^{-1} \left(\frac{\omega_c}{\gamma} \right) \right] \\
 & - \frac{\hbar e^{-\gamma\tau}}{m(\gamma^2 + \omega_c^2)} \left[\omega_c \cos(\omega_c \tau) + \gamma \sin(\omega_c \tau) \right] \\
 & + \frac{\hbar}{\pi m} \operatorname{Re} \left\{ \frac{1}{\gamma + i\omega_c} \left[e^{(\gamma + i\omega_c)t} E_1((\gamma + i\omega_c)t) + e^{-(\gamma + i\omega_c)t} E_1(-(\gamma + i\omega_c)t) \right] \right\}
 \end{aligned} \tag{5.27}$$

and

$$\begin{aligned}
 d_{12}(t) = & \operatorname{sign}(t) \frac{\hbar e^{-\gamma\tau}}{m(\gamma^2 + \omega_c^2)} \left[\gamma \cos(\omega_c \tau) - \omega_c \sin(\omega_c \tau) \right] \\
 & - \frac{\hbar}{\pi m} \operatorname{Im} \left\{ \frac{1}{\gamma - i\omega_c} \left[e^{(\gamma - i\omega_c)t} E_1((\gamma - i\omega_c)t) - e^{-(\gamma - i\omega_c)t} E_1(-(\gamma - i\omega_c)t) \right] \right\}, \tag{5.28}
 \end{aligned}$$

where $C = 0.577\dots$ is the Euler constant. The corresponding long-time behaviors of $d_{11}(t)$ and $d_{12}(t)$ are given by

$$\begin{aligned}
 d_{11}(t) = & \frac{2\hbar\gamma}{\pi m(\gamma^2 + \omega_c^2)} \ln \left(\tau \sqrt{\gamma^2 + \omega_c^2} \right) \\
 & + \frac{2\hbar}{\pi m(\gamma^2 + \omega_c^2)} \left[C\gamma + \omega_c \tan^{-1} \left(\frac{\omega_c}{\gamma} \right) \right] + O(t^{-2})
 \end{aligned} \tag{5.29}$$

and

$$d_{12}(t) = -\frac{4\hbar\gamma\omega_c}{\pi m(\gamma^2 + \omega_c^2)^2 t} + O(t^{-3}). \tag{5.30}$$

It is clear that the oscillatory terms with the cyclotron frequency are associated with the helical motions of a charged particle about the magnetic field. However, for times long enough, the time-dependence of $d_{11}(t)$ is not altered by the \vec{B} field, with only a reduced overall coefficient [131].

For later comparisons, we conclude this subsection by writing down the results for a free charged particle in a magnetic field, deduced from (5.19) and (5.20) by taking the limit $\gamma \rightarrow 0$:

$$d_{11}(t) = \frac{2\hbar}{m\omega_c} \coth\left(\frac{\hbar\omega_c}{2kT}\right) \sin^2\left(\frac{\omega_c t}{2}\right) \quad (5.31)$$

and

$$d_{12}(t) = \frac{2kTt}{m\omega_c} - \frac{\hbar}{m\omega_c} \coth\left(\frac{\hbar\omega_c}{2kT}\right) \sin(\omega_c t) . \quad (5.32)$$

C. Long-time dependence for frequency-dependent memory function

In this subsection we shall work with a class of the spectral distributions of the memory function popularized in the recent literature, namely [112],

$$\text{Re } \tilde{\mu}(\omega) = m\gamma_s \left(\frac{\omega}{\tilde{\omega}}\right)^{s-1} \theta(\Omega_c - \omega) , \quad (5.33)$$

where Ω_c is a cutoff frequency that is very large compared with all relevant frequency scales of the dissipative system, but much less than other characteristic cutoff frequencies such as the Drude, Debye, or Fermi frequencies, etc., depending on the physical model involved; and $\tilde{\omega}$ denotes an appropriate reference frequency so that γ_s has the usual dimension of frequency for all s . To avoid the pathological divergence of the memory function at zero time $\mu(0)$, s is restricted to be positive. The Fourier transform of the memory function $\tilde{\mu}(\omega)$ is connected with its spectral distribution by [82]

$$\tilde{\mu}(\omega) = -\frac{2i\omega}{\pi} \int_0^\infty d\omega' \frac{\text{Re } \tilde{\mu}(\omega' + i0^+)}{\omega'^2 - \omega^2 - i0^+} . \quad (5.34)$$

For convenience, we base the following calculations on the Laplace-integral representation rather than the Fourier-integral representation that has been employed so far. The two are related through an analytic continuation, e.g., $\tilde{\mu}(\omega) = \hat{\mu}(z = -i\omega)$, where, by convention, the Fourier transform is denoted by a tilde whereas the Laplace transform is marked by a hat. From (5.33) and (5.34), the corresponding Laplace transform of the memory function is given by

$$\begin{aligned}\hat{\mu}(z) = m\hat{\gamma}(z) &= \frac{2z}{\pi} \int_0^\infty d\omega \frac{\text{Re} \tilde{\mu}(\omega + i0^+)}{\omega^2 + z^2} \\ &= \frac{2m\gamma_s}{\pi s} \left(\frac{\Omega_c}{\tilde{\omega}} \right)^{s-1} \frac{\Omega_c}{z} F\left(1, \frac{s}{2}; 1 + \frac{s}{2}; -\frac{\Omega_c^2}{z^2}\right),\end{aligned}\quad (5.35)$$

where $\hat{\gamma}(z)$ is the associated friction coefficient introduced in (3.12), with its asymptotic expansion for small frequencies ($z \ll \Omega_c$) being [53]

$$\hat{\gamma}(z) = \begin{cases} \frac{\gamma_s}{\sin(\pi s/2)} \left(\frac{z}{\tilde{\omega}} \right)^{s-1} \left[1 + O\left(z/\Omega_c, (z/\Omega_c)^{2-s}\right) \right], & 0 < s < 2 \\ \frac{\gamma_2 z}{\pi \tilde{\omega}} \ln(1 + \Omega_c^2/z^2), & s = 2 \\ \frac{2\gamma_s}{\pi(s-2)} \left(\frac{\Omega_c}{\tilde{\omega}} \right)^{s-2} \frac{z}{\tilde{\omega}} \left[1 - \frac{\pi(s-2)/2}{\sin(\pi(s-2)/2)} \left(\frac{z}{\Omega_c} \right)^{s-2} + O(z^2/\Omega_c^2) \right], & 2 < s < 4 \\ \frac{2\gamma_s}{\pi(s-2)} \left(\frac{\Omega_c}{\tilde{\omega}} \right)^{s-2} \frac{z}{\tilde{\omega}} \left[1 + O(z^2/\Omega_c^2) \right], & s \geq 4 \end{cases}\quad (5.36)$$

The case of $\hat{\mu}(z) = (2/\pi)m\gamma_1 \tan^{-1}(\Omega_c/z)$ for $s=1$, from (5.35), corresponds to the Ohmic heat bath in the limit $\Omega_c/z \rightarrow \infty$, while the cases of $0 < s < 1$ and $s > 1$ have been referred to as sub-Ohmic and super-Ohmic, respectively [99].

For general frequency-dependent memory functions like the ones in (5.35), only the long-time behaviors of the system can be solved analytically in terms of known functions, with the dominant contributions coming from the small-frequency regions in the

integrals involved. Assembling (2.11), (3.4), (3.5), and (2.5) with ω_0 set to zero, we then find for the retarded Green's functions in the plane perpendicular to the magnetic field, in terms of the Laplace integral,

$$G_{11}(t) = \theta(t) \frac{1}{4\pi i m} \int_{\text{Br}} dz e^{z t} \left[\frac{1}{z^2 + z\hat{\gamma}(z) + i\omega_c z} + \frac{1}{z^2 + z\hat{\gamma}(z) - i\omega_c z} \right] \quad (5.37)$$

and

$$G_{12}(t) = \theta(t) \frac{1}{4\pi i m} \int_{\text{Br}} dz e^{z t} \left[\frac{1}{z^2 + z\hat{\gamma}(z) + i\omega_c z} - \frac{1}{z^2 + z\hat{\gamma}(z) - i\omega_c z} \right], \quad (5.38)$$

where the symbol Br stands for the Bromwich path, which goes upward parallel to the imaginary axis and with positive real part. The integrals in (5.37) and (5.38) for long times can be evaluated by expanding the fractions in the brackets about $z = 0$ and using Hankel's formula [130]

$$\frac{1}{2\pi i} \int_{\text{Br}} dz e^{z t} z^{-s} = t^{s-1} \Gamma^{-1}(s). \quad (5.39)$$

The calculation, though tedious, is straightforward, yielding

$$G_{11}(t) = \begin{cases} \frac{\sin(\pi s/2)}{m\gamma_s \Gamma(s)} (\tilde{\omega} t)^{s-1} \left[1 - \left(\frac{\omega_c}{\gamma_s} \right)^2 \sin^2 \left(\frac{\pi s}{2} \right) (\tilde{\omega} t)^{2s-2} \frac{\Gamma(s)}{\Gamma(3s-2)} + O((\tilde{\omega} t)^{s-2}) \right], & 0 < s < 1 \\ \frac{\gamma_1}{m(\gamma_1^2 + \omega_c^2)} + O((\Omega_c t)^{-1}), & s = 1 \\ \frac{1}{m\omega_c} \sin(\omega_c t) + O((\tilde{\omega} t)^{1-s}), & 1 < s < 2 \\ \frac{1}{m\omega_c} \sin \left[\frac{\omega_c t}{1 + (2\gamma_2/\pi\tilde{\omega}) \ln(\Omega_c t)} \right] + O((\tilde{\omega} t)^{-1}), & s = 2 \\ \frac{1}{m\omega_c} \sin \left(\frac{m}{m_r} \omega_c t \right) + O((\tilde{\omega} t)^{1-s}), & s > 2 \end{cases} \quad (5.40)$$

and

$$G_{12}(t) = \begin{cases} \frac{\omega_c \sin^2(\pi s/2)}{m \gamma_s^2 \Gamma(2s-1)} (\tilde{\omega} t)^{2s-2} \left[1 + O\left((\tilde{\omega} t)^{-1}, (\tilde{\omega} t)^{2s-2}\right) \right], & 0 < s < 1 \\ \frac{\omega_c}{m(\gamma_1^2 + \omega_c^2)} + O(\omega_c/\Omega_c t), & s = 1 \\ \frac{2}{m \omega_c} \sin^2\left(\frac{\omega_c t}{2}\right) + O\left((\tilde{\omega} t)^{-s}\right), & 1 < s < 2 \\ \frac{2}{m \omega_c} \sin^2\left[\frac{\omega_c t/2}{1 + (2\gamma_2/\pi \tilde{\omega}) \ln(\Omega_c t)}\right] + O\left(\ln(\Omega_c t)/(\tilde{\omega} t)^2\right), & s = 2 \\ \frac{2}{m \omega_c} \sin^2\left(\frac{m}{2m_r} \omega_c t\right) + O\left((\tilde{\omega} t)^{-s}\right), & s > 2 \end{cases} \quad (5.41)$$

where

$$m_r = m \left[1 + \frac{2}{\pi(s-2)} \gamma_s \tilde{\omega}^{1-s} \Omega_c^{s-2} \right] \quad (5.42)$$

is the renormalized mass for $s > 2$ [112].

The long-time dependence of the displacement correlation functions at finite temperatures may now be deduced from the first integral of (5.4)

$$d_{\rho\sigma}(t) = 2kT \int_0^t dt' G_{\rho\sigma}(t') \quad \text{for } t \rightarrow \infty \text{ and } T > 0. \quad (5.43)$$

Applied to (5.40) and (5.41), we then arrive at

$$d_{11}(t) = \begin{cases} \frac{2kT \sin(\pi s/2)}{m\gamma_s \tilde{\omega} \Gamma(s+1)} (\tilde{\omega} t)^s \left[1 - \left(\frac{\omega_c}{\gamma_s} \right)^2 \sin^2 \left(\frac{\pi s}{2} \right) (\tilde{\omega} t)^{2s-2} \frac{\Gamma(s+1)}{\Gamma(3s-1)} + O((\Omega_c t)^{-1}) \right], & 0 < s < 1 \\ \frac{2kT \gamma_1 t}{m(\gamma_1^2 + \omega_c^2)} + O(1), & s = 1 \\ \frac{4kT}{m\omega_c^2} \sin^2 \left(\frac{\omega_c t}{2} \right), & 1 < s < 2 \\ \frac{4kT}{m\omega_c^2} \left(1 + \frac{2\gamma_2}{\pi \tilde{\omega}} \ln(\Omega_c t) \right) \sin^2 \left[\frac{\omega_c t/2}{1 + (2\gamma_2/\pi \tilde{\omega}) \ln(\Omega_c t)} \right], & s = 2 \\ \frac{4kT m_r}{m^2 \omega_c^2} \sin^2 \left(\frac{m}{2m_r} \omega_c t \right), & s > 2 \end{cases} \quad (5.44)$$

and

$$d_{12}(t) = \begin{cases} \frac{2kT \omega_c \sin^2(\pi s/2)}{m\gamma_s^2 \tilde{\omega} \Gamma(2s)} (\tilde{\omega} t)^{2s-1} \left[1 + O((\tilde{\omega} t)^{-1}, (\tilde{\omega} t)^{2s-2}) \right], & 0 < s < 1 \\ \frac{2kT \omega_c t}{m(\gamma_1^2 + \omega_c^2)} + O(1), & s = 1 \\ \frac{2kT}{m\omega_c^2} [\omega_c t - \sin(\omega_c t)] + O((\tilde{\omega} t)^{1-s}), & 1 < s < 2 \\ \frac{2kT}{m\omega_c^2} \left\{ \omega_c t - \left(1 + \frac{2\gamma_2}{\pi \tilde{\omega}} \ln(\Omega_c t) \right) \sin \left[\frac{\omega_c t}{1 + (2\gamma_2/\pi \tilde{\omega}) \ln(\Omega_c t)} \right] \right\}, & s = 2 \\ \frac{2kT m_r}{m^2 \omega_c^2} \left[\frac{m\omega_c}{m_r} t - \sin \left(\frac{m}{m_r} \omega_c t \right) \right], & s > 2 \end{cases} \quad (5.45)$$

At zero temperature, we insert (5.40) and (5.41) into (5.15) and obtain, to leading-order terms in the long-time expansion,

$$d_{11}(t) = \begin{cases} \frac{1}{\bar{s} \sin(\pi/\bar{s})} \frac{2\hbar}{m\tilde{\omega}} \phi^{1/\bar{s}} - \frac{(3-\bar{s})(3-2\bar{s})}{\bar{s}^3 \sin(3\pi/\bar{s})} \frac{\hbar \omega_c^2}{m\tilde{\omega}^3} \phi^{3/\bar{s}}, & 0 < s < 1 \\ \frac{2\hbar \gamma_1 \ln(t)}{\pi m(\gamma_1^2 + \omega_c^2)}, & s = 1 \\ \frac{\hbar}{(s-1)m\omega_c}, & 1 < s < 2 \\ \frac{\hbar}{m\omega_c}, & s \geq 2 \end{cases} \quad (5.46)$$

where $\phi \equiv (\tilde{\omega}/\gamma_s) \sin(\pi s/2)$ and $\bar{s} \equiv 2 - s$; and

$$d_{12}(t) = \begin{cases} O(t^{-3}), & 0 < s < \frac{1}{2} \\ \frac{\hbar \omega_c}{\pi m \gamma_{1/2}^2 \tilde{\omega} t}, & s = \frac{1}{2} \\ \frac{\hbar \omega_c}{m \gamma_s^2 \Gamma(2s-1)} \sin^2\left(\frac{\pi}{2}s\right) \tan[(1-s)\pi] (\tilde{\omega} t)^{2s-2}, & \frac{1}{2} < s < 1 \\ -\frac{4\hbar \gamma_1 \omega_c}{\pi m (\gamma_1^2 + \omega_c^2)^2 t}, & s = 1 \\ -\frac{\hbar}{m \omega_c} \sin(\omega_c t), & 1 < s < 2 \\ -\frac{\hbar}{m \omega_c} \sin\left[\frac{\omega_c t}{1 + (2\gamma_2/\pi \tilde{\omega}) \ln(\Omega_c t)}\right], & s = 2 \\ -\frac{\hbar}{m \omega_c} \sin\left(\frac{m}{m_r} \omega_c t\right), & s > 2 \end{cases} \quad (5.47)$$

Since a magnetic field does not affect particle motions parallel to it, the results for $G_{33}(t)$ and $d_{33}(t)$ are the same as those in the one-dimensional case [53,112]. We list them here for completeness and for later comparison with the results for motions in the plane normal to the magnetic field:

$$G_{33}(t) = \begin{cases} \frac{\sin(\pi s/2)}{m \gamma_s \Gamma(s)} (\tilde{\omega} t)^{s-1} \left[1 + O((\Omega_c t)^{-1}, (\Omega_c t)^{s-2})\right], & 0 < s < 2 \\ \frac{\pi}{2m \gamma_2} \frac{\tilde{\omega} t}{\ln(\Omega_c t)} \left[1 + O(\ln^{-1} t)\right], & s = 2 \\ \frac{t}{m_r} \left[1 + \frac{m}{m_r} \frac{\gamma_s \tilde{\omega}^{1-s} t^{2-s}}{\Gamma(4-s) \sin(\pi(s-2)/2)} + O((\Omega_c t)^{-2})\right], & 2 < s < 4 \\ \frac{t}{m_r} + O((\Omega_c t)^{-1}), & s \geq 4 \end{cases} \quad (5.48)$$

$$d_{33}(t) = \begin{cases} \frac{2kT \sin(\pi s/2)}{m\gamma_s \tilde{\omega} \Gamma(s+1)} (\tilde{\omega}t)^s + O(t^{s-1}, t^{2s-2}), & 0 < s < 2 \\ \frac{\pi kT}{2m\gamma_2 \tilde{\omega} \ln(\Omega_c t)} (\tilde{\omega}t)^2 + O((\tilde{\omega}t)^2 / \ln^2(\Omega_c t)), & s = 2 \\ \frac{kT}{m_r} t^2 + O(t^{4-s}), & s > 2 \end{cases} \quad (5.49)$$

and

$$d_{33}(t)|_{T=0} = \begin{cases} \frac{2}{\bar{s} \sin(\pi/\bar{s})} \frac{\hbar}{m\tilde{\omega}} \phi^{1/\bar{s}}, & 0 < s < 1 \\ \frac{2\hbar}{\pi m\gamma_1} \ln(t), & s = 1 \\ \frac{\sin^2(\pi(2-s)/2)}{\cos(\pi(2-s)/2) \Gamma(s)} \frac{\hbar}{m\gamma_s} (\tilde{\omega}t)^{s-1}, & 1 < s < 2 \\ \frac{\pi^2 \hbar}{4m\gamma} \frac{\tilde{\omega}t}{\ln^2(t)}, & s = 2 \\ \frac{1}{\cos(\pi(2-s)/2) \Gamma(4-s)} \frac{\hbar m\gamma_s}{m_r^2 \tilde{\omega}^2} (\tilde{\omega}t)^{3-s}, & 2 < s < 3 \\ \frac{2\hbar m\gamma_3}{\pi m_r^2 \tilde{\omega}^2} \ln(t), & s = 3 \\ \bar{d}_\infty, & s > 3 \end{cases} \quad (5.50)$$

where $\phi \equiv (\tilde{\omega}/\gamma_s) \sin(\pi s/2)$ and $\bar{s} \equiv 2-s$; and

$$\bar{d}_\infty = \frac{2\hbar}{\pi} \int_0^\infty dz \left[\frac{1}{m(z^2 + z\hat{\gamma}(z))} - \frac{1}{m_r z^2} \right] \quad (5.51)$$

is a constant depending on high-frequency, as well as low-frequency, properties of the memory function.

A comparison of these results for a charged quantum particle moving perpendicular or parallel to an external magnetic field enables us to see the influence of the magnetic field on the Brownian motion. For the retarded Green's functions at long times in the sub-Ohmic case ($0 < s < 1$), with the magnetic field \bar{B} set along the z axis, $G_{11}(t)$ is the

same as $G_{33}(t)$ to the leading-order term in t . In the Ohmic case ($s = 1$), as shown in Sec. IV, $G_{11}(t)$ is qualitatively the same as $G_{33}(t)$, with only a smaller mobility coefficient reduced by the magnetic field. In the super-Ohmic case ($s > 1$), however, $G_{11}(t)$ is completely different from $G_{33}(t)$ which ever increases with t . The particle responds to a constant driving force with a bounded simple harmonic oscillation in the plane normal to \bar{B} . In that plane, the damping now effectively vanishes for long times, except for the special case of $s = 2$ arising from the corresponding nonanalytic logarithmic term in (5.36) for $\hat{\gamma}(z)$, and for $s > 2$, the free particle's mass m is replaced by its renormalized mass m_r and the quantity $m\omega_c/m_r = eB/m_r c$ in Eqs. (5.40)–(5.45) and (5.47) is merely the cyclotron frequency for a particle with the renormalized mass m_r .

As for the long-time dependence of the displacement correlation functions in the sub-Ohmic case ($0 < s < 1$), $d_{11}(t)$ has the same subdiffusive behavior as $d_{33}(t)$ at non-zero temperatures. On the other hand, the long-time constant limit of $d_{11}(t)$ is reduced by the magnetic field from that of $d_{33}(t)$ at $T = 0$. In the Ohmic case ($s = 1$), the magnetic field simply decreases the diffusion coefficient in the expression for $d_{11}(t)$ [111,131]. For $s > 1$, in contrast to the unbounded growth at long times (except for $s > 3$ at $T = 0$) of $d_{33}(t)$, $d_{11}(t)$ approaches a constant at zero temperature while displays bounded oscillations, except for $s = 2$ again, at nonzero temperatures.

VI. Summary and Discussion

We have considered the problem of calculating the retarded Green's functions and the symmetrized position correlation functions for a charged quantum oscillator linearly coupled to a heat bath, and in the presence of a constant homogeneous magnetic field. The retarded Green's functions are shown, as in the linear-response theory, to be related to the commutators (i.e., antisymmetrized correlation functions) of the position operators at different times, which are c-number quantities here owing to the linear nature of the coupling between particle and bath in the IO model. In correspondence, the retarded Green's

functions studied here are temperature-independent and are connected with the symmetrized position correlation functions by the fluctuation–dissipation (FD) theorem. For linear systems as are discussed here, all higher-order correlation functions can be factorized into summations of simple pair-correlation functions due to the Gaussian properties of the underlying stochastic processes [82].

We have started off by examining some general properties of the generalized susceptibility tensor of the dynamical system involved, which in turn have enabled us to reach two general conclusions about the position autocorrelation functions (dispersions) of the magnetic system in an arbitrary heat bath. In addition to the transversal dispersions of a charged quantum particle, the free energy of such a system has also been shown to decrease monotonically with increasing intensity of the magnetic field, hence indicating the diamagnetism of the system even in the presence of a physical heat bath. The generality of these theorems stems from the fact that, because of the neutrality of the independent oscillators implied in the IO model, the magnetic field enters into the GLE only through the Lorentz-force term so that the external field and the dissipation do not affect each other. It may be of interest to note in passing a similar theorem on the magnetoconductivity of metals that states under rather general assumptions that if an external magnetic field has no bearing on scattering mechanisms, then the electric conductivity of metals is a monotonically nonincreasing function of the magnitude of the magnetic field [159].

We have also investigated the quantum diffusion of a charged Brownian particle in a uniform magnetic field for a variety of heat baths. As in the nonmagnetic case, well-separated time scales, essential for the interpretation in terms of a standard Brownian motion, emerge only in the high-temperature (classical) regime. In the opposite limit of low temperature, the interplay between quantum and thermal fluctuations prevails, leading to long-time tails of the form t^{-2} in the time correlation functions [160]. For the

Ohmic heat bath, both the friction and the Lorentz force terms depend linearly on the instantaneous velocity of the charged particle. Accordingly, the functional dependencies on time of both the retarded Green's functions and the displacement correlation functions are qualitatively the same as those for a free particle; they are unchanged by the magnetic field, with only the overall coefficients reduced by a field-dependent cofactor for motions normal to it. Hence, a static magnetic field can not confine a charged particle coupled to an Ohmic heat bath, not even at absolute zero temperature. It only slows down the transverse diffusion [131]. For the sub-Ohmic case where damping dominates at low frequencies (or, equivalently, at long times), an initially localized state remains localized at zero temperature, even without an external confining potential, because of a finite variance $\sigma(t)$ here [112]: $\sigma(t) \equiv \langle (x - \langle x \rangle_t)^2 \rangle_t = \sigma(0) - d(t)/2 + \hbar^2 G^2(t)/4\sigma(0)$. Thereby the transverse localization length $\sigma^{1/2}(t \rightarrow \infty)$ is shorter than the longitudinal one. For the super-Ohmic case, the magnetic field dominates at long times. As a result, the traverse localization lengths are bounded except for the case of $s = 2$ at $T \neq 0$, whereas the longitudinal one is infinite. Therefore an initially localized state will eventually spread out along the direction of the magnetic field.

We conclude the discussion by pointing out that the method and results presented here may be useful in studying magnetic properties such as, e.g., the diamagnetic susceptibility, magnetoconductivity, and Hall coefficient for a two-dimensional (2D) system of charged particles in the dissipative (or incoherent) regime $\hbar\tau^{-1} \gg kT_0$, where τ is the inelastic scattering life time and T_0 is the bare degeneracy temperature. Two prototypes of quasi-two-dimensional system are the normal state in cuprate superconductors and the degenerate Fermi gas in inversion layers at semiconductor surfaces in the presence of strong disorder (associated with the quantized Hall effect). It has been argued that quantum statistics (both Bose and Fermi) present only quantitative corrections in the dissipative regime [161], and it is well known that for a system of interacting fermions, two

body interactions do not alter the amplitude and period of the de Haas–van Alphen oscillations as well as the total magnetic moment [162]. Therefore the GLE approach developed for the problem of a single charged Brownian particle might be applicable to such systems as well.

Appendix A

Let's denote the inverse matrix of $\alpha_{\rho\sigma}(\omega)$ by $D_{\rho\sigma}(\omega)$. Then we have [155]

$$D_{\rho\sigma}(\omega) = \lambda\delta_{\rho\sigma} + i\frac{e}{c}\omega\epsilon_{\rho\sigma\eta}B_{\eta}, \quad (\text{A1})$$

which, by definition, is related to $\alpha_{\rho\sigma}(\omega)$ through the equations

$$D_{\rho\eta}(\omega)\alpha_{\eta\sigma}(\omega) = \delta_{\rho\sigma} \quad (\text{A2})$$

and

$$\alpha_{\rho\eta}(\omega)D_{\eta\sigma}(\omega) = \delta_{\rho\sigma}, \quad (\text{A3})$$

where the Kronecker delta function $\delta_{\rho\sigma}$ is unity for $\rho = \sigma$, and zero otherwise.

From (A1) and (2.5), we find

$$D_{\rho\sigma}^*(\omega) - D_{\sigma\rho}(\omega) = 2i\delta_{\rho\sigma}\omega\text{Re}\tilde{\mu}(\omega). \quad (\text{A4})$$

Multiplying (A4) by $\alpha_{\rho\mu}(\omega)\alpha_{\sigma\nu}^*(\omega)$ and using (A2), we obtain (2.7) and, similarly, (2.8) by multiplying (A4) by $\alpha_{\nu\sigma}(\omega)\alpha_{\mu\rho}^*(\omega)$ with the aid of (A3).

Appendix B

Since $1/\lambda \equiv \alpha^{(0)}(\omega)$ is simply the generalized susceptibility for a one-dimensional oscillator, $-iz/\lambda(z) = -iz\alpha^{(0)}(z)$ is a positive real function for $K > 0$ [83], and thus its real part everywhere in the UHP is positive [82]

$$\text{Re}[-iz/\lambda(z)] > 0 \quad \text{for } \text{Im } z > 0. \quad (\text{B1})$$

Let's now suppose that

$$\lambda(z) = \pm m\omega_c z \quad (\text{B2})$$

for some z in the UHP. Then we would get

$$-iz/\lambda(z) = \mp i/m\omega_c, \quad (\text{B3})$$

which contradicts (B1). Therefore (B2) has no roots in the UHP. It follows that $\alpha_{\rho\sigma}(\omega)$, from (2.3), has no poles in the UHP.

Appendix C

To prove (2.10), we start by calculating the work done by an external, c-number force \tilde{f} (aside from the magnetic field) in a complete cycle on an otherwise isolated system [82]

$$\begin{aligned} W &= \int_{-\infty}^{\infty} dt f_{\rho}(t) \langle v_{\rho}(t) \rangle \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \tilde{f}_{\rho}(\omega) \langle \tilde{v}_{\rho}(-\omega) \rangle, \end{aligned} \quad (\text{C1})$$

where the second equality is obtained by using the Parseval theorem [169], $v_{\rho}(t)$ is the velocity operator of the particle, and $\tilde{f}(t)$ is assumed to be arbitrary except for the requirement that it vanish at both the distant past and the distant future, and where tilde denotes the Fourier transform as usual, e.g.,

$$\tilde{v}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} v(t). \quad (\text{C2})$$

From (C2), one can easily see that

$$\tilde{v}_{\rho}(\omega) = -i\omega \tilde{r}_{\rho}(\omega). \quad (\text{C3})$$

Putting (C3) and (2.2), with \tilde{f} added to \tilde{F} , in (C1) and averaging out the random force \tilde{F} gives

$$W = \frac{i}{2\pi} \int_{-\infty}^{\infty} d\omega \omega \alpha_{\mu\nu}^*(\omega) \tilde{f}_{\mu}(\omega) \tilde{f}_{\nu}^*(\omega) , \quad (C4)$$

where we have used the reality condition on $\tilde{v}(\omega)$: $\tilde{v}(-\omega) = \tilde{v}^*(\omega)$. Forming complex conjugate of (C4) and interchanging the dummy indices μ and ν , one then finds

$$W = -\frac{i}{2\pi} \int_{-\infty}^{\infty} d\omega \omega \alpha_{\nu\mu}(\omega) \tilde{f}_{\mu}(\omega) \tilde{f}_{\nu}^*(\omega) . \quad (C5)$$

Assembling (C4), (C5), (2.7), (2.2), and (C3), one finally obtains

$$\begin{aligned} W &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \omega \frac{1}{2i} [\alpha_{\nu\mu}(\omega) - \alpha_{\mu\nu}^*(\omega)] \tilde{f}_{\mu}(\omega) \tilde{f}_{\nu}^*(\omega) \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \omega^2 \operatorname{Re} \tilde{\mu}(\omega) \sum_{\sigma} |\alpha_{\sigma\mu}(\omega) \tilde{f}_{\mu}(\omega)|^2 \\ &= \frac{1}{\pi} \int_0^{\infty} d\omega \operatorname{Re} \tilde{\mu}(\omega) \sum_{\sigma} |\langle \tilde{v}_{\sigma}(\omega) \rangle|^2 , \end{aligned} \quad (C6)$$

which is positive as demanded by the second law of thermodynamics.

Equation (C4) may also be written as

$$W = \frac{1}{\pi} \int_0^{\infty} d\omega \omega \left\{ \operatorname{Im} \alpha_{\mu\nu}(\omega) \operatorname{Re} [\tilde{f}_{\mu}(\omega) \tilde{f}_{\nu}^*(\omega)] - \operatorname{Re} \alpha_{\mu\nu}(\omega) \operatorname{Im} [\tilde{f}_{\mu}(\omega) \tilde{f}_{\nu}^*(\omega)] \right\} , \quad (C7)$$

where we have used the fact that, due to the reality conditions on $\alpha_{\mu\nu}(\omega)$ and $\tilde{f}_{\mu}(\omega)$, $\operatorname{Re} \alpha_{\mu\nu}(\omega)$ and $\operatorname{Im} \alpha_{\mu\nu}(\omega)$, as well as $\operatorname{Re} \tilde{f}_{\mu}(\omega)$ and $\operatorname{Im} \tilde{f}_{\mu}(\omega)$, are even and odd functions of ω , respectively. Since $\tilde{f}_{\mu}(\omega)$ are arbitrary other than the boundary conditions $\lim_{\omega \rightarrow \pm\infty} \tilde{f}_{\mu}(\omega) = 0$, $\tilde{f}_{\mu}(\omega)$ ($\mu = 1, 2, 3$) may well be chosen all real (and thus even functions of ω). Then the integrand in (C7), according to (C6), must be positive for all ω

$$\operatorname{Im} \alpha_{\mu\nu}(\omega) \tilde{f}_{\mu}(\omega) \tilde{f}_{\nu}(\omega) = \operatorname{Im} \alpha_{\mu\nu}^s(\omega) \tilde{f}_{\mu}(\omega) \tilde{f}_{\nu}(\omega) > 0 \quad \text{for } \omega > 0 , \quad (C8)$$

where $\alpha_{\mu\nu}^s(\omega)$, given by (3.2), is the symmetric part of $\alpha_{\mu\nu}(\omega)$. Hence $\text{Im } \alpha_{\mu\nu}^s(\omega)$ must be a positive definite matrix for all $\omega > 0$, and (2.10) readily follows as a corollary.

Appendix D

The free energy of a charged quantum oscillator linearly coupled to a neutral heat bath, and in a magnetic field, defined as the free energy of the composite system of the oscillator interacting with the heat bath minus that of the heat bath itself, assumes the form [155]

$$F_O(T, B) = \frac{1}{\pi} \int_0^\infty d\omega f(\omega, T) \text{Im} \left\{ \frac{d}{d\omega} \ln [\det \alpha(\omega + i0^+)] \right\}, \quad (\text{D1})$$

where $f(\omega, T)$ is the free energy (including zero-point energy) of a free oscillator of frequency ω :

$$f(\omega, T) = kT \ln [2 \sinh(\hbar\omega/2kT)], \quad (\text{D2})$$

and where

$$\det \alpha(\omega) = [\det D(\omega)]^{-1} = \left\{ \lambda \left[\lambda^2 - (e/c)^2 \bar{B}^2 \omega^2 \right] \right\}^{-1} \quad (\text{D3})$$

is the determinant of the matrix $\alpha_{\rho\sigma}(\omega)$ given in (2.3).

Since the heat bath is neutral, the magnetic moment M of the charged oscillator is related to the free energy $F_O(T, B)$ through the equation [170]

$$M = -\frac{\partial}{\partial B} F_O(T, B). \quad (\text{D4})$$

Substituting (D1)–(D3) in (D4) and integrating by parts once gives

$$\begin{aligned}
M &= B \frac{\hbar e^2}{\pi c^2} \int_0^\infty d\omega \omega^2 \coth\left(\frac{\hbar\omega}{2kT}\right) \text{Im}\left[\lambda^2 - (e/c)^2 B^2 \omega^2\right]^{-1} \\
&= B \left(\frac{e}{c}\right)^2 \frac{\hbar}{2\pi i} \int_{-\infty}^\infty d\omega \omega^2 \coth\left(\frac{\hbar\omega}{2kT}\right) \left[\lambda^2 - (e/c)^2 B^2 \omega^2\right]^{-1}, \quad (\text{D5})
\end{aligned}$$

where we have used in the last line the reality condition on the quantity in the brackets. Before we move on, it would be of interest to check the classical limit of (D5). Expanding $\coth(\hbar\omega/2kT)$ for small \hbar and exploiting the analyticity of the integrand in the UHP (cf. Appendix B), we get

$$M = B \left(\frac{e}{c}\right)^2 \frac{kT}{\pi i} \int_{-\infty}^\infty d\omega \omega \left[\lambda^2 - (e/c)^2 B^2 \omega^2\right]^{-1} = 0, \quad (\text{D6})$$

which is expected on account of the quantum nature of magnetism (the Bohr–van Leeuwen theorem) [171].

The integration in (D5) may be performed by closing the contour in the UHP and by using the partial-fractional expansion of $\coth(z)$ [167]

$$\coth(z) = \sum_{n=-\infty}^{\infty} \frac{1}{z + in\pi}. \quad (\text{D7})$$

The resulting serial expression of M is

$$M = -2kTB \left(\frac{e}{mc}\right)^2 \sum_{n=1}^{\infty} \frac{v_n^2}{\hat{\lambda}^2(v_n) + (v_n \omega_c)^2} < 0, \quad (\text{D8})$$

where $v_n = (2\pi kT/\hbar)n$ are again the Matsubara frequencies. Hence, the magnetic moment due to the orbital motion of a charged oscillator is still diamagnetic, unaltered by the presence of an arbitrary heat bath. The same holds for a charged Brownian particle as one takes the limit $\omega_0^2 \rightarrow 0$ in (D8).

For an Ohmic heat bath at zero temperature, the magnetic moment of a charged oscillator can be calculated explicitly by using the result for the free energy [155]:

$$M = -\frac{\hbar e^2 B}{2\pi m^2 c^2 b} \left\{ \frac{\gamma^2/4 + (b+a)/2}{\sqrt{(b+a)/2}} \tan^{-1} \left(\frac{2}{\gamma} \sqrt{\frac{b+a}{2}} \right) - \frac{\gamma^2/4 - (b-a)/2}{2\sqrt{(b-a)/2}} \ln \left[\frac{\gamma/2 + \sqrt{(b-a)/2}}{\gamma/2 - \sqrt{(b-a)/2}} \right] \right\}, \quad (\text{D9})$$

where the quantity within the braces is positive [cf. Eqs. (4.8) and (4.9) of Ref. 155]. For a charged Brownian particle, this reduces in the limit $\omega_0^2 \rightarrow 0$ to

$$M = -\frac{\hbar e}{\pi m c} \tan^{-1} \left(\frac{\omega_c}{\gamma} \right). \quad (\text{D10})$$

IV

SUMMARY

In Chapter I of this dissertation, we have presented a review of the theory of stochastic processes, with strong emphasis on pedagogical aspects. We have given a survey of the basic concepts and properties of stochastic processes for both the classical and quantum-mechanical systems. Since its birth at the beginning of this century, the theory of stochastic processes has become quite mature, especially in the classical domain. It has found applications in almost every discipline of science. However, many problems still remain, particularly regarding the quantum dissipative systems.

In Chapter II of this dissertation, we have applied the generalized quantum Langevin equation (GLE) approach to some of the problems of interest in the literature, whereas Chapter III is devoted to the quantum dissipative systems of charged particles in the presence of a magnetic field.

In Chapter II, Brownian motion in a general heat bath is investigated by using the GLE. The solutions to the equation (and to the more general one describing a harmonically bound Brownian particle) are used to calculate the correlation between the displacement and the random force, which is shown to reproduce the classical results in the high-temperature limit. Memory effects of the environment are exemplified by consideration of the blackbody radiation heat bath. Furthermore, the mean square displacement of a damped quantum harmonic oscillator is calculated, permitting one to reach general conclusions regarding the effects of dissipation on the localization of the oscillator within the framework of the GLE.

In Chapter III of this dissertation, we have shown that the 3D equation of motion for a charged quantum particle moving in a static external magnetic field as well as a potential, and coupled linearly to a heat bath, can still be cast in the form of a GLE, with the influence of the magnetic field solely represented by a quantum version of the Lorentz-force term. The generality and transparency of the results allow them to easily be applied to cases of physical interest, like the case of a blackbody radiation heat bath.

Various physical properties, including the symmetrized position correlation functions and the free energy, of the dissipative system of a charged harmonic oscillator placed in a constant, homogeneous magnetic field can then be expressed in terms of the generalized susceptibility tensor, which in turn may be obtained from the corresponding GLE. Explicit calculations are made for the Ohmic and the blackbody radiation heat baths.

Furthermore, the mean square displacements for the special case of a free charged Brownian particle are evaluated for an Ohmic heat bath at zero temperature. The complication of the combined effects of both dissipation and magnetic field is discovered consequently.

Finally, we have studied the retarded Green's functions and the symmetrized position correlation functions for an isotropic spatial harmonic potential. The retarded Green's functions are shown, as in the linear-response theory, to be related to the commutators (i.e., antisymmetrized correlation functions) of the position operators at different times, which are c-number quantities for linear models. We next examine some general properties of the generalized susceptibility tensor of the dynamical system involved to reach two general conclusions about the position autocorrelation functions (dispersions) of the magnetic system in an arbitrary heat bath. In addition, the free energy of such a system has also been shown to be generally diamagnetic in an arbitrary physical heat bath. We have also investigated the quantum diffusion of a charged Brownian particle in

a uniform magnetic field for a variety of heat baths. As in the nonmagnetic case, the standard Brownian motion only emerges in the high-temperature (classical) regime. In the opposite limit of low temperature, the interplay between quantum and thermal fluctuations prevails, leading to the familiar power-law long-time tails in the symmetrized position correlation functions. For the Ohmic heat bath, both the friction and the Lorentz-force terms depend linearly on the instantaneous velocity of the charged particle. Accordingly, the functional dependencies on time of both the retarded Green's functions and the displacement correlation functions are qualitatively the same as those for a free particle; they are unchanged by the magnetic field, with only the overall coefficients reduced by a magnetic-field-dependent factor for motions orthogonal to it. For the super-Ohmic case, the magnetic field dominates at long times. As a result, the transverse localization lengths are bounded, whereas the longitudinal one is infinite. Therefore an initially localized state will eventually spread out along the direction of the magnetic field.

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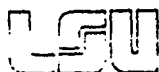
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APPENDIX
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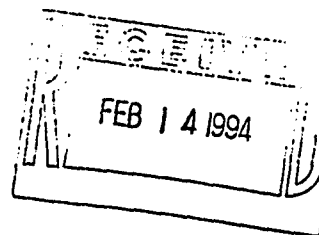
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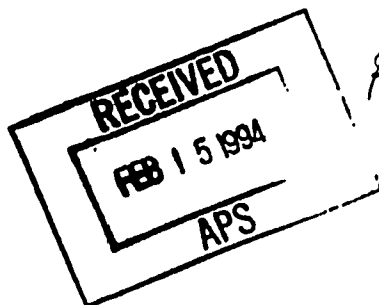
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VITA

Xiao Liang Li was born in Shanghai, the People's Republic of China on April 8, 1963. He attended the Associated High of East China Normal University from 1977 to 1981. In the fall of 1981, he enrolled at Fudan University in Shanghai, China and received a Bachelor of Science degree in Physics four years later. He was admitted in 1986 as a graduate student in the Department of Physics and Astronomy at Louisiana State University and currently is a candidate for the Doctor of Philosophy degree in physics.

DOCTORAL EXAMINATION AND DISSERTATION REPORT

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Xiao Liang Li

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Physics

Title of Dissertation:

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Major Professor and Chairman

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